TOPSPIN 1.3

Installation Guide

for Windows XP

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Chapter 1

Introduction

1.1 About this manual

This manual is the TOPSPIN installation Guide for Microsoft Windows XP and describes the installation of the TopSpin 1.3 under Microsoft Windows XP.

It is available:

- as a hard copy 'TOPSPIN for Windows XP: Installation Guide'
- as `pdf` file on the TOPSPIN DVD
- as TOPSPIN Online Help: click ***Help*** → ***Installation Guide***
- as the up to date version on the Bruker web-server:

  `http://www.bruker-biospin.de/NMR/nmr-softw/passwd/docu/index.html`

- Note that this manual does not contain the TOPSPIN Release letter. That is a separate document which is not available as a hard copy but delivered as `pdf` and `text` files on the TOPSPIN DVD and also on the Bruker web-server (you can find it at the same URL as the Installation Guide)

  `http://www.bruker-biospin.de/NMR/nmr-softw/passwd/docu/index.html`

This manual is subdivided into an introduction and three main parts. It depends on

your local demands which of these are necessary for you at the moment.

The first part shows how to install and configure TOPSPIN and some essential additional software packages. It is recommended to follow the instructions step by step.

Part two describes the scratch installation of Windows XP and some configuration steps for Windows XP, the network and printers. If you want to install Bruker BioSpin TOPSPIN on a PC which is already in use, you can skip this part.

In the last part, you can find some additional information for working with Windows XP and TOPSPIN and also some tips for troubleshooting.

Note that all text-messages and graphics shown in this book are taken from the current version of the respective software products. Small differences to other versions are possible but generally speaking they should be very similar.

If you have any comments or suggestions, or if you find any errors in this manual, please do not hesitate to contact us at:

nmr-software-support@bruker-biospin.de

1.2 Conventions

`Bold-Courier`: Windows XP commands to be entered from the keyboard

Bold-Times: Windows XP commands, applications or buttons to be clicked with the mouse

`Bold-Courier-Italics`: TOPSPIN commands to be entered from the keyboard

Bold-Times-Italic: TOPSPIN commands to be clicked with the mouse

`Courier`: a file name or directory name

`Courier Small Italics`: response of the system

`Courier Small`: the contents of a file

Times italics: any name which is not a file name e.g. hostnames, usernames etc.

< >: place holder

1.3 Hardware and software requirements for TOPSPIN

1.3.1 Operating system requirements

The following operating systems are tested and supported for TOPSPIN 1.3.

Linux	Windows
Red Hat Enterprise Linux WS 3	Windows 2000 / Windows XP

Any other operating systems might also work but because TOPSPIN 1.3 was not tested there, usage of not supported operating system is at one's own risk.

1.3.2 Special PC Hardware requirements

To run TOPSPIN 1.3 we recommend the following computer hardware:

- PC with CPU Clock ≥ 1 GHz
- Memory ≥ 512 MB
- Video (graphics)-card memory: 64 MB [1]
- Ethernet card (to control a spectrometer, it is essential to have a second ethernet card)
- Mouse with 3-button possibilities
- DVD device[2]

If your hardware does not meet these requirements, TOPSPIN might still run but with a much lower performance.

Furthermore, we recommend setting the display resolution to 1280*1024 or higher.

The Installation was tested on a 'hp workstation xw4100' PC with a 'NVIDIA Quadro4 380 XGL' graphics card and two 'Broadcom NetXtreme Gigabit Ethernet' cards.

1.3.3 Spectrometer requirements

TOPSPIN 1.3 is released for datastations and Avance-AQS, Avance-AQX/AQR

1. It is recommend not to use shared memory graphics, because in some cases memory problems could be observed.
2. TOPSPIN 1.3 is delivered on DVD's with "-r" format.

spectrometers.

For upgrade possibilities of your spectrometer with TOPSPIN 1.3, please get in touch with your local Bruker representative.

Hardware components that are TOPSPIN version or operating system dependent are listed below. Components that are not listed here do not need an upgrade for TOPSPIN 1.3.

Please note that AQS and AQX/AQR components cannot be interchanged.

If your Avance spectrometer does not meet the above specifications, please get in touch with your local Bruker representative for your upgrade options.

1.3.4 Avance systems with AQS rack

- **•CCU**

Windows, independent of the TOPSPIN Version	
CCU	**required minimum EC level**
CCU 10 (part # H9503)	requires no specific EC level
CCU 11 [1] (part # H9503V1)	**00** (recommended **01**)

1. Note that CCU 11 also exists for AQX/AQR spectrometers.

LINUX, independent of the TOPSPIN Version	
CCU	**required minimum EC level**
CCU 10 (part # H9503) EC level 00 to 19	**06**
CCU 10 (part # H9503) EC level > 19	**22**
CCU 11 [1] (part # H9503V1)	**00** (recommended **01**)

1. Note that CCU 11 also exists for AQX/AQR spectrometers.

- **FCU 3**

FCU 3	required minimum EC level
part # H5822 (64k memory)	**04**
part # H9598 (256k memory)	**02**

- **RCU**

RCU	required minimum EC level
RCU 1/2 (part # Z003678)	requires no specific EC level
RCU 1/3 (part # Z022488)	requires no specific EC level

Note: RCUs with EC level 06 of the AQX/AQR rack can also be used in an AQS rack

Multiple Receiver RCU	required minimum EC level
RCU 1/2 (part # Z052488)	requires no specific EC level
RCU 2/4 (part # Z062488)	requires no specific EC level
RCU 3/4 (part # Z072488)	requires no specific EC level
RCU 4/4 (part # Z082488)	requires no specific EC level
RCU 1/5 (part # Z003206)	requires no specific EC level
RCU 2/5 (part # Z003207)	requires no specific EC level
RCU 3/5 (part # Z003208)	requires no specific EC level
RCU 4/5 (part # Z003209)	requires no specific EC level

- **TCU 3**

TCU	required minimum EC level
part # H5813 with EC level between 00 and 19	**09**
part # H5813 with EC level between 20 and 29	**28**
part # H5813V1	requires no specific EC level
part # H5813F2	requires no specific EC level
part # H5813F3	requires no specific EC level

1.3.5 Avance systems with AQX/AQR rack

- **•CCU**

Windows	
CCU	**required minimum EC level**
CCU 04 (part # H2552)	**04**
CCU 05 (part # H2570) EC level 00 to 19	**05**
CCU 06 (part # H2570) EC level 20 to 29	**24**
CCU 08 (part # H2570) EC level 40 to 49	**43**
CCU 09 (part # H2570)	requires no specific EC level
CCU 11 [1] (part # H2570V1)	requires no specific EC level

1. Note that CCU 10 does not exist for AQX/AQR spectrometers. Further note that CCU 11 also exists for AQS spectrometers.

LINUX	
CCU	**required minimum EC level**
CCU 04 (part # H2552)	**05**
CCU 05 (part # H2570) EC level 00 to 19	**06**
CCU 06 (part # H2570) EC level 20 to 29	**26**
CCU 08 (part # H2570) EC level 30 to 39	**38**
CCU 08 (part # H2570) EC level 40 to 49	**46**
CCU 09 (part # H2570) EC level 50 to 59	**55**
CCU 09 (part # H2570) EC level 60 to 69	**62**
CCU 11 [1] (part # H2570V1)	requires no specific EC level

1. Note that CCU 10 does not exist for AQX/AQR spectrometers. Further note that CCU 11 also exists for AQS spectrometers.

- **TCU**

TCU	required minimum EC level
TCU 1 main board (part # H5811 or 5812)	**03**
TCU 0 main board (part # H2558)	**07**
TCU extention board (part # H2562)	**03**
TCU extention board (part # H2562) in DMX/DRX with > 5 channels	**20**

- **RCU**

RCU	required minimum EC level
RCU 1/1 (part # Z002488) 64kB SRAM & 1MB DRAM	**06**
RCU 1/2 (part # Z012488) 256kB SRAM & 2MB DRAM	**06**
RCU 1/3 (part # Z022488) 1MB SRAM & 2MB DRAM	**06**

Note: 'normal' RCUs and multiple receiver RCUs should not be mixed!

Multiple Receiver RCU	required minimum EC level
RCU 1/2 (part # Z052488)	requires no specific EC level
RCU 2/4 (part # Z062488)	requires no specific EC level
RCU 3/4 (part # Z072488)	requires no specific EC level
RCU 4/4 (part # Z082488)	requires no specific EC level
RCU 1/5 (part # Z003206)	requires no specific EC level
RCU 2/5 (part # Z003207)	requires no specific EC level
RCU 3/5 (part # Z003208)	requires no specific EC level
RCU 4/5 (part # Z003209)	requires no specific EC level

- **FCU**

FCU0 64k memory: part # H2556 64k memory: part # H2554	required minimum EC level
FCU0: for use without cortab	**04**
FCU0: for DSX without use of cortab	**05**
FCU0: for use with cortab with EC level between 00 and 19	**07**
FCU0: for use with cortab with EC level $\geq$ 20	**21**

Tomo FCU	required minimum EC level
part # T5565 (64k memory) for use without cortab	**00**
part # T5565 (64k memory) for use with cortab	**02**
part # T6765 (256k memory) for use with or without cortab EC level between 00 to 19	**00**
part # T6765 (256k memory) for use with or without cortab EC level between 20 to 29	**21**

1.3.6 Software requirements

!
- Microsoft Windows XP (SP2) or Windows 2000 (SP4) for TOPSPIN $\geq$ 1.3 [1]
- on DVD: 'TOPSPIN 1.3'
  - TOPSPIN
  - Flexlm License Manager [see Chapter 7]
- For spectrometer control:
  - Hummingbird NFS Server Version 7.1 (*CD*: TOPSPIN NT Toolkit) [see Chapter 4]
- For NMR-GUIDE:
  - Internet Explorer $\geq$ 6.x (*CD:* Microsoft Windows XP)
- For TOPSPIN Online Help and NMR GUIDE
  - A PDF viewer (e.g. Adobe Acrobat Reader [see Chapter 5])

1. TopSpin requires a NTFS filesystem on the partition where the Topspin is installed and a NTFS filesystem on all partitions where Topspin data are stored [see chapter 14.1].

1.4 Important Windows configurations

This Installation Guide for TOPSPIN refers to the following configurations for Windows XP. Several functions (e. g. Control Panel, Start menu, Windows Explorer) can be configured in a *Classic view*-mode or *Category view*-mode (Windows XP style). These modes are not only different in style. They can be different in the way commands are entered.

1.4.1 Configure the Start Menu

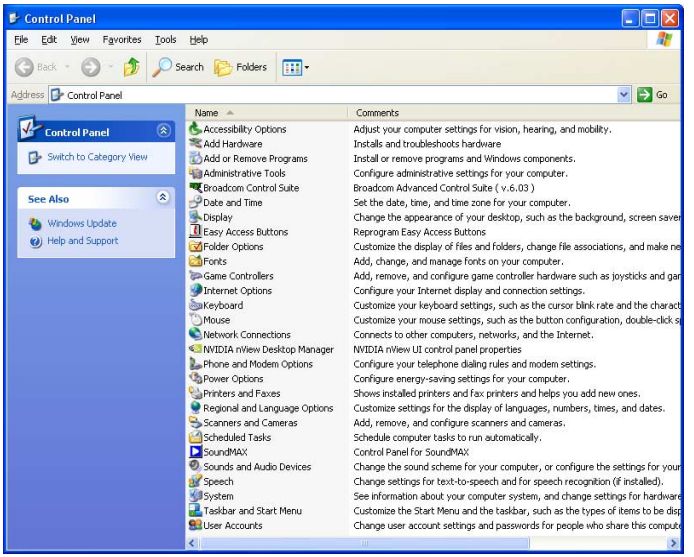
For this manual the Start Menu is configured in the Windows XP style.

- Click the RIGHT mouse button on the Taskbar → click **Properties**
- Click **Start Menu** → click **Start Menu** → click **OK**

1.4.2 Configure the Control Panel and the Windows Explorer

For this manual the Control Panel and the Windows Explorer are configured in the *Classic View* style.

- Click on the left side on *Switch to Classic View*


Control Panel
File Edit View Favorites Tools Help
Back Search Folders
Address Control Panel
Go
Control Panel
Switch to Category View
See Also
Windows Update
Help and Support
Name
Comments
Accessibility Options
Adjust your computer settings for vision, hearing, and mobility.
Add Hardware
Installs and troubleshoots hardware
Add or Remove Programs
Install or remove programs and Windows components.
Administrative Tools
Configure administrative settings for your computer.
Broadcom Control Suite
Broadcom Advanced Control Suite (v.6.03)
Date and Time
Set the date, time, and time zone for your computer.
Display
Change the appearance of your desktop, such as the background, screen saver
Easy Access Buttons
Reprogram Easy Access Buttons
Folder Options
Customize the display of files and folders, change file associations, and make ne
Fonts
Add, change, and manage fonts on your computer.
Game Controllers
Add, remove, and configure game controller hardware such as joysticks and gar
Internet Options
Configure your Internet display and connection settings.
Keyboard
Customize your keyboard settings, such as the cursor blink rate and the charact
Mouse
Customize your mouse settings, such as the button configuration, double-click s
Network Connections
Connects to other computers, networks, and the Internet.
NVIDIA nView Desktop Manager
NVIDIA nView UI control panel properties
Phone and Modem Options
Configure your telephone dialing rules and modem settings.
Power Options
Configure energy-saving settings for your computer.
Printers and Faxes
Shows installed printers and fax printers and helps you add new ones.
Regional and Language Options
Customize settings for the display of languages, numbers, times, and dates.
Scanners and Cameras
Add, remove, and configure scanners and cameras.
Scheduled Tasks
Schedule computer tasks to run automatically.
SoundMAX
Control Panel for SoundMAX
Sounds and Audio Devices
Change the sound scheme for your computer, or configure the settings for your
Speech
Change settings for text-to-speech and for speech recognition (if installed).
System
See information about your computer system, and change settings for hardware
Taskbar and Start Menu
Customize the Start Menu and the taskbar, such as the types of items to be disp
User Accounts
Change user account settings and passwords for people who share this compute

Chapter 2

Express Installation and Configuration of TOPSPIN

2.1 About this chapter

This chapter gives a brief description of how to install Bruker BioSpin's TOPSPIN.

This chapter is directed to users who would like to install TOPSPIN 1.3 on a PC, on which XWIN-NMR or a version of TOPSPIN is already installed and configured correctly. Therefore this chapter provides an overview and provides not information on all aspects of configuring Windows XP and TOPSPIN.

For more details on the installation see chapter 6.4.

For more details on the ***TOPSPIN*** commands like ***cf***, ***expinstall***, etc. please refer to the description of this command in the Acquisition Reference manual.

2.2 Installing TOPSPIN

The main decision you have to make during installation is where do you want to install the new TopSpin version. If you a have previous NMR SUITE or TOPSPIN installation on this PC available, you can either:

- install the new version in parallel to the previous one

  or

- install the new version in the same directory as the previous one

The installation in parallel has the advantage, that the previous version remains unchanged. After a parallel installation you can start working with the new version and if you want to go back to the previous version for whatever reasons you can just start and reuse it.

The installation of TOPSPIN 1.3 offers an automatic import of your individual configuration of a previous version, so that there is no advantage to install the new version in the same directory as the old one.

1. Log in as a Local Administrator

2. Close ALL WINDOWS on the desktop

3. Insert the DVD 'TOPSPIN *1.3*' .

4. Start of the installation

- If the automatic start of the DVD is enabled, the window described in the next step appears automatically, go to step 5
- If this window of the next step does not appear automatically, autorun is probably switched off (see chapter 10.3) or open the Windows Explorer, go to the DVD device and double-click `install.cmd` [1].

5. The windows *Welcome to the TOPSPIN Setup* will appear: → Click **Next**

6. A window *Release Letter TOPSPIN* will appear:

a) Please read the NMR Release letter! You can find there all information about news and bug fixes of the current version.

b) Close the Release Letter by clicking the **X** button in the upper right corner

- Select the destination directory for TOPSPIN.

  a) Accept the default destination

  b) or browse to another destination.

  - Enter an installation path which does not exists so far, e. g. ***C:\Bruker\topspin1.3***
  - or browse to another existing installation path.

1. Please note that there is also a file called 'install' on the DVD. This file is the installation script for Linux, under Windows you have to click on the file 'install.cmd'

- Click **OK**

- Click **Next**

7. A window *Select the setup type* will appear:

a) Select the setup type. Do one of the following:

- Select *Data Processing, Acquisition and Automation* if you want to use TOPSPIN for spectrometer control. This will install **Diskless** automatically.
- Select *Data Processing* if you want to use TOPSPIN for data processing.
- *Customized setup* (allows components selection) if you want to install selected programs only.

  A window 'Product selection' will appear. Select the packages which you want to install (note that DISKLESS is only required if your PC controls a spectrometer or you want to configure it like this.

b) Click **Next**

8. If *Data Processing, Acquisition and Automation* were selected in step 8, a window *Information* will appear:

If the spectrometer (CCU) is booted, please shut it down. To do this, run telnet, connect to spect, login as root, type /etc/init 5 (You can activate the Windows Start menu with Ctrl-Esc)

If the PC is not yet connected to a spectrometer or if the CCU is not booted [1] you can immediately → Click **OK**

If your PC is currently connected to a spectrometer and the CCU is booted:

a) Press the keys **CTRL+ESC** (to open the Start menu)

b) Click **Start** → **All Programs** → **Accessories** → **Command Prompt**

c) Enter: **`rsh spect -l root /etc/init 5`**

→ this will shut down the CCU

d) Enter: **`exit`**

e) Close the window *Information* by clicking **OK**

Note: The CCU is now either down or switched off and should be turned on again at the end of this procedure.

1. Note that during a first time installation of the TOPSPIN the CCU can not be booted.

9. A window '*Question*' will appear if Windows XP Service Pack 2 is installed and enabled on your system. If you click **Yes** on the installation configure the firewall[1] for you.[2]

10. A window '*Select Components*' will appear. You can either import no spectrometer configuration, or browse for a spectrometer configuration or select one of the configurations you get offered within this window [3].

- Click **Next**

11. A window '*Set NMR Super User*' will appear:

a) Do one of the following:

- Accept the default NMR Superuser (Administrator) or
- Enter a special user for this purpose, e.g. named *nmrsu* or
- Enter any other user

Under Windows the username must be the name of an existing user. For further details check chapter 6.2.

b) Click **Next**

12. A window '*Password Input*' will appear [4] (for more details about this feature see chapter 6.2):

a) Do one of the following:

- Type in the NMR ADMINISTRATION PASSWORD
- Re-enter the NMR ADMINISTRATION PASSWORD

b) Click **Next**

→ The installation of TOPSPIN will start now.

13. A window '*Setup is complete*' will appear:

- You will be asked if you want to restart the computer:

a) Click **Yes I want to restart my computer now**

---

1. The firewall must be configured to enable spectrometer access.
2. If you click on **No** an Administrator can do it any time later, running *<topspin-home>\prog\bin\Utilities\Miscellaneous\setfirewal.cmd (see chapter 8.8).*
3. The installation process will offer all configurations which are available in the TOPSPIN / XWIN-NMR installation that are defined in the registry.
4. Certain commands like ***cf*** and ***expinstall*** ask for the NMR ADMINISTRATION PASSWORD.

b) Click **Finish** (to reboot the computer)

14. After the PC has booted up, press the reset button on the CCU or turn it on with the key if it was switched off. Don't forget to execute ***cf*** and ***expinstall*** (if necessary; see chapter 2.3).

The following information is for the *Customized setup:*

! • It is strongly recommended to accept the default path for the flexLM installation: `'C:\flexlm'` ! If you choose a user defined path, it may cause some problems with other applications using the FlexLM.

2.3 Configuring TOPSPIN

The idea of this chapter is to give you some guidelines to configure TOPSPIN for using it on a workstation for data processing, or for operating a spectrometer. We do not discuss the commands in detail here. For a full description refer to the TOPSPIN manuals.

Start TOPSPIN:

- Click the icon TOPSPIN on the desktop, or
- Click **Start** → **All Programs** → **Bruker TOPSPIN** → **TOPSPIN<vers.>**

After the first startup of TOPSPIN a window 'LICENSE' will appear:

a) Please read the license agreement for Bruker TOPSPIN !

b) If you agree, please click **I Accept**.

After the first startup of TOPSPIN a window 'Configuration check' will appear.

You have the possibility to configure the software (depending upon the hardware of your spectrometer). If you do this, you are probably in one of five situations:

1. You want to configure a processing-only-PC with a default configuration on a datastation → go to chapter 2.3.1 (see also chapter 8.1.3)

2. You have just installed the software in a new directory and the old spectrometer configuration of the software is still known to the new version → go to chapter 8.1.1

3. You want to configure a processing-only-PC like your spectrometer-PC, so you have the spectrometer configuration on another computer → go to chapter 8.1.2

4. You have to configure the software on a new hard disk without a backup of the spectrometer configuration, so you have no configuration files → go to chapter 8.1.4
5. You have a new spectrometer hardware component, so you have no configuration file → go to chapter 8.1.5

If you would like to take over the configuration of an existing XWIN-NMR or TOPSPIN installation into TOPSPIN 1.3, please check chapter 8.2.

2.3.1 If you want to use a default configuration on a datastation

A default configuration can be used on a PC that is used for processing only. It is automatically performed (no ***cf*** required) during the installation of TOPSPIN on a new computer, a new disk or in a new TOPSPIN installation directory. The default configuration name is *Bruker_default_av500* and corresponds to an Avance 500 MHz spectrometer.

For data processing, the automatic default configuration is sufficient. If, however, you want to use AU programs, you must execute ***expinstall*** and select *Installation for Datastation (Default)*.

For further details please refer to the respective chapters (see chapter 8.1.2).

2.3.2 If your PC controls a spectrometer:

1. Be sure that the spectrometer is booted (see chapter 6.4 and also 15.5.3)
2. Open a dataset
   - Type ***new*** and create a new dataset.
   - You can also select a dataset (e.g. *exam1d_1h*) acquired with another TOPSPIN or XWIN-NMR version
3. Enter ***cf*** (The command ***cf*** now configures the software according to the hardware of your spectrometer.)
   a) A window will appear:
   Password request. Please enter the NMR administration password

   Type in the NMR ADMINISTRATION PASSWORD. Click **OK**.

   b) A window will appear:
   Spectrometer configuration: ...

Most likely you will select an existing configuration and press **Edit** to confirm this configuration.

c) A window will appear:
Edit configuration. ...

The selected configuration is displayed. Choose whether to configure it as a spectrometer or datastation. Choose the type of your spectrometer e.g. ***AVANCE*** → **ENTER**. Check or type in the 1H frequency of the magnet e. g. ***500.13*** → **ENTER**. Use the debug mode only in case of trouble-shooting.

d) A window will appear:
Specify the channel to which external devices are connected. The RS232/485 channel for external devices-Table appears.

Check if the tty-numbers of the hardware components are set correctly.

e) A window '*Additional configuration*' will appear:
Security check. Enable peak power check (POWCHK).

- Choose the options if you want to use this security options. *Powchk* and *Pulchk* require special probes and *cortab*. If in doubt contact your local Bruker representative, please.

Sample changer configuration. Should the Sample Changer control the Lift? (yes/no)

- The answer depends on how the air flow is connected, normally you will answer: ***yes*** → **ENTER**

Delay between SX and next command [sec]?

- Type in the length of the delay e. g. ***10*** → **ENTER**

f) The *nuclei-table* appear

Check if the frequency of the nuclei are set correctly. If in doubt click ***Restore*** then click ***Save***

g) A window 'Edit spectrometer configuration will appear:
Check if the preamplifier connections are set correctly and click ***Save***..

h) The results of ***cf*** appears in a text window. Check this list carefully and compare the result with an list from an earlier configuration (if available) click ***Print*** and store the paper output with your other spectrometer documentation, then click ***OK***. *These data are saved in <TOPSPINHOME>/conf/instr/<spect>/uxnmr.info.*

If during 'cf' an error message occurs that invites you to do a firmware update check chapter 15.5

After finishing ***cf*** the window '*config*' will appear showing a list of configuration steps. You will be asked for the NMR ADMINISTRATION PASSWORD several times:

- Continue with ***expinstall***
  a) Type in the NMR ADMINISTRATION PASSWORD and **ENTER**
  b) Click **Next** if you either have not modified Bruker BioSpin Parameter files, AU-programs and Pulse-programs or if you have archived them in a different directory. Your individual Parameter files, AU-programs and Pulse-programs etc. that are named different to the original Bruker BioSpin files will not be destroyed during the installation.
  c) A window appears: Check *Installation for Spectrometer* → Click ***Next***
  d) In the appearing window: Check *the required system* → Click ***Next***
  e) In the appearing dialog box: Select the spectrometer configuration name → Click ***Next***
  f) In the appearing dialog box: Check the items you want to install or, accept the default selection → Click ***Next***
  g) In the appearing dialog box: Select the default printer and plotter and the desired paper format → Click ***Next***
  h) In the appearing window: Enter the desired spectrometer frequency, acquisition mode and pre-scan-delay or, accept the default values → Click ***Next***
  i) In the appearing information box: Check the configuration selection and, if it is correct → Click ***Finish***
  While Expinstall will be executed, you can configure the next configuration programs.
- Continue with ***edsolv***
  Check the list of lock solvents → click ***Save*** if it is correct → Click ***Close***
- Continue with ***edhead***
  Select the current probe → click ***Define as current probe*** → Click ***Exit***
- Continue with ***edprosol***
  Check the parameters for your observed nuclei, and if necessary change and/or recalculate them → Click ***Save*** to store to disk → Click ***Exit***

- Continue with ***edlock***

  Check the lock table values (field, lock phase, ...), change them and click ***Save*** if necessary, otherwise click ***Abort***

- Continue with ***edscon***

  Check the spectrometer constants, change them and click ***Save*** if necessary, otherwise click ***Cancel***

After ***cf***, ***expinstall***,... have finished insert a sample and make sure that you can lock on the lock solvent. Type ***ii*** and read with ***rpar*** a standard Bruker BioSpin parameter file (e. g. 'rpar PROTON all'), type ***getprosol***, ***rga*** and ***wobb*** and collect a normal ^{1}H NMR spectrum.

2.3.3 If you want to configure a processing-PC like your spectrometer-PC:

If the PC does not control a spectrometer but is used in connection with a particular spectrometer, e.g. for setting up experiments, processing and or plotting, you should configure it as that spectrometer (see FAQ 210 on www.bruker-biospin.de) (see chapter 8.1.2).

Part I

TOPSPIN - Installation and Configuration

Chapter 3

General Installing Information

3.1 Installation order

A complete new installation on a PC connected to a spectrometer involves the following steps:

1. Installing Windows XP (see chapter 11.1)
2. Installing Windows XP Service Pack (see chapter 11.2)
3. Installing the Graphics driver (see chapter 11.3)
4. Installing NFS Server (see chapter 4.3) [1]
5. Installing TOPSPIN (see chapter 6.4)
6. Configuring NFS Server (see chapter 6.6)
7. Installing TOPSPIN license (see chapter 7.2)
8. Configuring of TOPSPIN for spectrometer control (see chapter 8.1.1)
9. Configuring the network (see chapter 13)
10. Installing a printer (see chapter 14)

1. Note for Windows XP SP2 users with enabled firewall: If you have installed the NFS server after TOPSPIN, you have to execute `setfirewall.cmd` again (see chapters 4.5 and 8.8)!

11. Installing a PDF viewer (see chapter 5)

If your PC is already in use, steps 1 to 3 are probably already done. In that case, you can start with step 4.

Chapter 4

Installing NFS Server

4.1 TOPSPIN NT Toolkit CD

The Bruker BioSpin *TOPSPIN NT Toolkit*-CD (for Windows XP) contains the Hummingbird NFS Server 7.1.

The version of the NFS Server for Windows XP that is currently supported is 7.1: If this is already installed, you can skip this chapter.

The NFS Server is available on the *TOPSPIN NT Toolkit*-CD that can be ordered from Bruker BioSpin, part number H9437W0.

Please contact your sales representative for the price of the NFS Server. Alternatively, you can contact NFS manufacturer Hummingbird [1] for information on how to obtain NFS 7.1 or how to upgrade from an earlier version.

4.2 Preparing for the TOPSPIN NT Toolkit installation

The NFS Server is required if your PC controls a spectrometer; it makes the DISKLESS package available for the CCU.

1. See www.hummingbird.com

Before you install the NFS Server:

- Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
- Enter **`ipconfig /all`**

and check if the network is installed. If it is not, install the network as described in chapter 13.

4.3 Installing NFS Server

IMPORTANT:

- before installing NFS you must configure TCP/IP (see chapter 13.1)
- If your installation fails with following error message:

  ```
  CreatThisService::Createservice:Error # [997]
  ```

  Your network-adapter has no link to the network. Establish a link to the network or install the

  `NWlink IPX/SPX/NetBIOS Compatible Transport Protocol:`

  a) Click **Start** → **Control Panel** → **Network Connections** → Right-click **Local Area Connection xxx**

  b) Click **Properties** → **Install...** → **Protocol** → **Add**

  c) The *`Select Network Protocol`*-menu will appear after some seconds. → Click **NWlink ...** → **OK**

  d) After some seconds the Properties-menu will reappear: → Click **Close**

If another version is installed, remove it according to chapter 10.2, reboot the computer and install a newer version.

If you have the Hummingbird NFS Maestro CD be aware of the following. An Evaluation CD, will only work for a limited amount of time. Please check if your delivery contains another NFS Maestro CD. If it does, this is probably the full version. If it does not, you probably ordered an Evaluation CD. Please use the full version if you have one! Now insert the NFS Maestro CD.

4.3.1 Installing NFS 7.1 from the Bruker BioSpin *TOPSPIN NT Toolkit*-CD

1. Log in as a Local Administrator

2. Insert the CDROM *TOPSPIN NT Toolkit*
3. Double-click the icon **My Computer**
4. A window '*My Computer*' will appear:
   - Double-click the CDROM icon
5. A window showing the contents of the CDROM will appear:
   - Double-click the icon **setupNFS** or **setupNFS.cmd**
6. A window '*Hummingbird Master Setup*' will appear:
   - Click **Install NFS Maestro Server**

     This window will change to the subtitle '*Installation Type*'
     - Click **Personal Installation**
     - A window '*Chose Setup Language*' will appear:
       - Choose **English (USA)** (this description is written for the English one)
       - Click **OK**
     - A window '*Hummingbird Setup Wizard*' will appear and display several progress bars. Finally it shows:

       The Hummingbird Setup Wizard will install Hummingbird NFS Maestro Server on your computer ...
       - Click **Next**
     - A window '*License Agreement*' will appear:
       - Click **I accept ...** → Click **Next**
     - A window '*Customer Information*' will appear. Insert the appropriate information or leave the information unchanged (it is important that this application will be installed for anyone who uses this computer):
       - Click **Next**
     - A window '*Destination Folder*' will appear:
       - Click **Next**
     - A window '*Setup Type*' will appear:
       - Click **Typical** → Click **Next**
     - A window '*Ready to Install the Program*' will appear:
       - Click **Install**
     - A window '*Installing Hummingbird NFS Maestro Server*' will appear showing a progress bar

- A window '*Hummingbird Setup Wizard Completed*' will appear:
  - Click **Finish**
- Back in the window '*Hummingbird Master Setup*':
  - Click **Back** → Click **Exit**

7. Remove the CDROM

The certificate '*Proof of license*' is delivered with each TOPSPIN NT Toolkit CD. It proves that you have an official copy of the Hummingbird NFS Server. Please keep this certificate!

4.4 Configuring the NFS Server for spectrometer control

Before you can configure the NFS Server (described in chapter 6.6) you must first install packages on the TOPSPIN DVD, particularly the DISKLESS package (see chapter 6.4).

4.5 Firewall configuration for the NFS Server

If you have enabled the firewall under Windows XP SP2, you have to configure the firewall for the NFS Server. This can be done automatically during the TOPSPIN installation or later while executing the setfirewall.cmd (<topspin-home>\prog\bin\Utilities\Miscellaneous\setfirewal.cmd) (see chapter 8.8).

Note: If you have installed the NFS Server after the TOPSPIN installation, you have to configure the firewall again!

Chapter 5

Installing a PDF viewer.

5.1 When do I need a PDF viewer?

A PDF viewer is required for displaying the TOPSPIN Online Help and for parts of the NMR-GUIDE. A PDF viewer is not installed automatically as a part of TOPSPIN. Bruker BioSpin recommends to use the Adobe Acrobat Reader. The Acrobat Reader is available from Adobe as a download:

http://www.adobe.com

Chapter 6

Installing TOPSPIN

6.1 Preparing for the TOPSPIN installation

Before you install TOPSPIN:

1. TOPSPIN can only be installed on a NTFS filesystem, not on a FAT file system. However, you can convert FAT to NTFS as described in chapter 12.1.2.
2. Before you proceed, make sure you are logged in as a Local Administrator. If you are not sure about this, press **Ctrl-Alt-Del** (just as for a logon). The popup screen tells you the current user-id. If you are indeed logged in as a Local Administrator, click **Cancel**. Otherwise click **logoff** and then log on as an Administrator.
3. Click **Start** → **All Programs** → **Accessories** → **Command Prompt**

   enter: `ipconfig /all`

   and check if the local network is configured. If it is not, configure the network as described in chapter 13.

If your PC controls a spectrometer:

1. Click **Start** → **All Programs**

and check if you see the entry NFS Maestro. If it does not appear, install NFS Maestro Server as described in chapter 4.3.

2. Click **Start** → **All Programs** → **Accessories** → **Command Prompt**

   enter: **`ipconfig /all`**

   and check if the second Ethernet adapter is configured. If it is not, configure it as described in chapter 13.

6.2 NMR SUPERUSER and NMR ADMINSTRATION PASSWORD

TOPSPIN offers a complete new password check for the configuration tools of TOPSPIN. During the TOPSPIN installation, you are prompted to define:

1. The username for the so called NMR SUPERUSER. If you choose an NMR SUPERUSER other than Administrator make sure that this user exists. The NMR SUPERUSER can be Administrator (this is the default) or any other user (can also be a Domain account). We recommend installing a special user for this purpose, e.g. a user named *nmrsu*. This user does not need any special permissions under Windows; standard access permissions are sufficient.
   - After the installation, the NMR SUPERUSER is the owner of all TOPSPIN program files. Logging in as this user allows you to remove these files, change file permissions etc. The name of the NMR SUPERUSER will be stored in the file: `<TOPSPINHOME>/conf/nmrsuperuser`
2. the NMR ADMINISTRATION PASSWORD to be used for TOPSPIN configuration commands. This password can be freely chosen and is not connected to any user. It is asked for by TOPSPIN commands like ***`cf`***, ***`expinstall`*** etc. The encrypted NMR ADMINISTRATION PASSWORD is stored in the file:

   `<TOPSPINHOME>/conf/nmradminpassword`

! Note: The NMR SUPERUSER login password and the NMR ADMINISTRATION PASSWORD have different purposes and are totally independent. Changing one of them does not affect the other.

With the information about the NMR ADMINISTRATION PASSWORD and NMR SUPERUSER TOPSPIN is ready to be configured. The NMR ADMINISTRATION PASSWORD will be asked for every time a configuration type command is entered. If this password is typed in correctly, the command will be

executed independent of which user is logged in the operating system. As a result all newly created configuration files will be owned by the user that was logged in at the time the configuration command was executed. Any other user can modify the configuration during his login session, just by knowing the correct NMR ADMINISTRATION PASSWORD. This is possible because all configuration files are read- and writeable for everybody, but TOPSPIN will not write them without the correct NMR ADMINISTRATION PASSWORD!

TOPSPIN also offers a so-called *Security Mode*. With this feature all configuration files are only read- and writeable for the NMR SUPERUSER.

6.2.1 How to change the NMR ADMINSTRATION PASSWORD

The *installnmr* script can be used to change the NMR ADMINISTRATION PASSWORD and the NMR SUPERUSER. If it is called with the option '-secure', it changes the permissions in a way, that only the NMR SUPERUSER can execute the configuration commands and the resulting files are readable and writable only for him, all other users have read-only permissions.

To change the NMR ADMINISTRATION PASSWORD, you have to:

1. Login as NMR Superuser or Administrator
2. Double click on the icon 'Bruker Utilities' on the desktop.

   A window Bruker Utilities will appear
3. Double click on the command prompt

   Note: It is not possible to use a 'normal' windows command prompt, because in this 'special' command prompt of 'Bruker Utilities' there are several parameters and path entries defined.
4. Type in:

   perl\bin\perl prog\bin\installnmr <TOPSPINHOME> <NMRSUPERUSER>

   If you installed TOPSPIN in the default directory and you want to use the user 'nmrsu' as NMR SUPERUSER, you have to type in

   ```
   perl\bin\perl prog\bin\installnmr C:\Bruker\TopSpin nmrsu
   ```
5. Enter the old password and new password as requested.

6.2.2 How to define a new NMR ADMINSTRATION PASSWORD

To define a new NMR ADMINISTRATION PASSWORD, for example because

you have forgotten it, you have to:

1. Login as the Administrator
2. Open a Windows Command Prompt
3. Delete the file <x>\conf\nmradminpassword
4. Enter:

```
perl\bin\perl prog\bin\installnmr <TOPSPINHOME> <NMRSUPERUSER>
```

5. Enter new password as requested.

6.3 Packages on the TOPSPIN DVD

1. TOPSPIN: Acquisition and processing software
2. TOPSPIN PLOT EDITOR: Object oriented WYSIWYG plot editor (automatically installed as part of the TOPSPIN package)
3. ICON-NMR: Icon-driven interface for Routine Spectroscopy and Automation
4. NMR-GUIDE: Web-browser based teaching and training program
5. DISKLESS: Spectrometer CCU operating system
6. NMR-SIM: Program for numerical simulation of NMR experiments
7. AMIX-Viewer: new multiple object viewer (requires a separate license)
8. AURELIA: Analysis of 2D/3D/4D NMR data (requires separate license)
9. GLP: Program for 'Good Laboratory Practice' tests (requires separate license)
10. FLEXLM: License manager required for starting TOPSPIN programs.
11. GNU TOOLS: System tools required by TOPSPIN.
    (automatically installed as part of the TOPSPIN package)
12. PERL: language interpreter required for certain TOPSPIN commands.
    (automatically installed as part of the TOPSPIN package)

6.4 Installing TOPSPIN

This chapter describes the installation of the TOPSPIN as a local Administrator, using a local NMR Superuser account. Chapter 13.6 describes additional steps which must be taken if you want to install the TOPSPIN in a Domain.

The main decision you have to make during installation is where do you want to install the new TopSpin version. If you have a previous NMR SUITE or TOPSPIN installation on this PC available, you can either:

!

- install the new version in parallel to the previous one

  or

- install the new version in the same directory as the previous one

The installation in parallel has the advantage, that the previous version remains unchanged. After a parallel installation you can start working with the new version and if you want to go back to the previous version for whatever reasons you can just start and reuse it.

The installation of TOPSPIN 1.3 offers an automatic import of your individual configuration of a previous version, so that there is no advantage to install the new version in the same directory as the old one.

1. Log in as a Local Administrator

2. Close ALL WINDOWS on the desktop

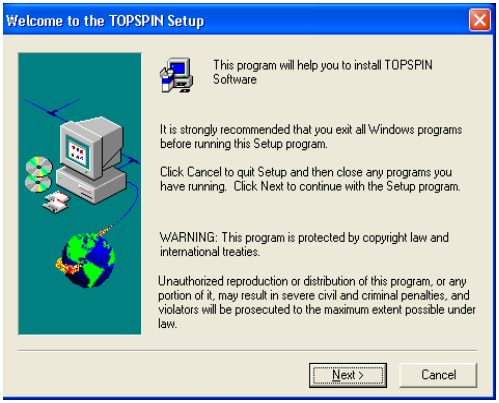
3. Insert the DVD 'TOPSPIN *1.3*' .

4. Start of the installation

- If the automatic start of the DVD is enabled, the window described in the next step appears automatically, go to step 5
- If this window of the next step does not appear automatically, autorun is probably switched off (see chapter 10.3) or open the Windows Explorer, go to the DVD device and double-click `install.cmd` [1].

5. The windows *Welcome to the TOPSPIN Setup* will appear: → Click **Next**

1. Please note that there is also a file called 'install' on the DVD. This file is the installation script for Linux, under Windows you have to click on the file 'install.cmd'


Welcome to the TOPSPIN Setup
This program will help you to install TOPSPIN Software
It is strongly recommended that you exit all Windows programs before running this Setup program.
Click Cancel to quit Setup and then close any programs you have running. Click Next to continue with the Setup program.
WARNING: This program is protected by copyright law and international treaties.
Unauthorized reproduction or distribution of this program, or any portion of it, may result in severe civil and criminal penalties, and violators will be prosecuted to the maximum extent possible under law.
Next >
Cancel

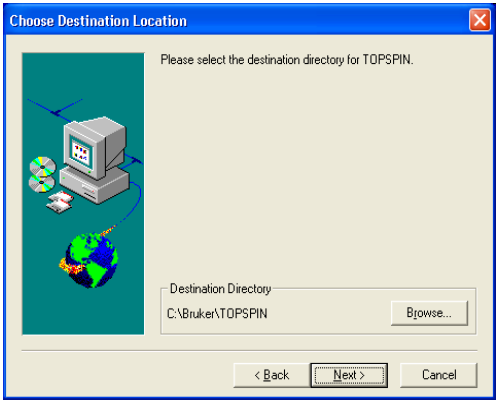
6. A window *Release Letter TOPSPIN* will appear:

rellet.txt - Notepad
File Edit Format View Help
R E L E A S E L E T T E R
T O P S P I N 1.3
Chapter 1
Introduction
1.1 About Topspin development
With Topspin 1.3 supports the full range of Avance spectrometers
Avance-AQS and Avance-AQX/AQR. This means Avance-AQX/AQR
spectrometers, including DMX/DRX/DSX/DPX can now be upgraded from
Xwin-nmr to Topspin.

a) Please read the NMR Release letter! You can find therein all information about news and bug fixes of the current version.

b) When you have finished reading the Release Letter, close the Release Letter by clicking the **X** button in the upper right corner.

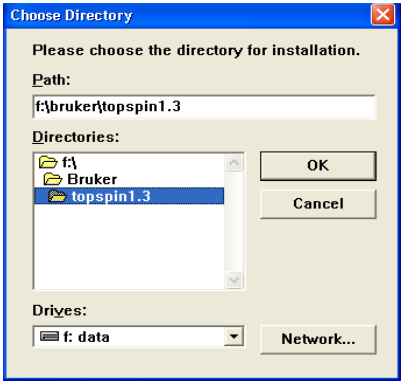
7. A window *Choose Destination Location* will appear:



- Select the destination directory for TOPSPIN.

  a) Accept the default destination

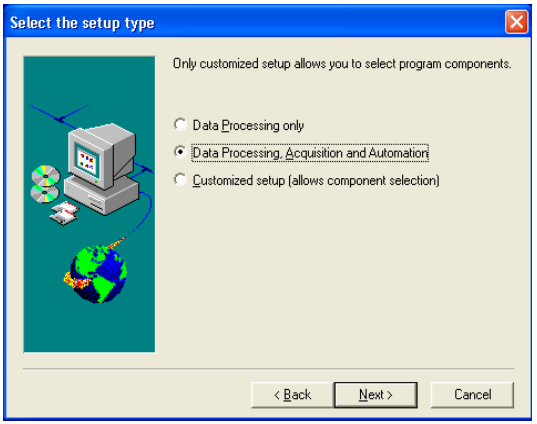
  b) or browse to another destination.



  - Enter an installation path which does not exists so far, e. g. ***C:\Bruker\topspin1.3***
  - or browse to another existing installation path.
  - Click **OK**

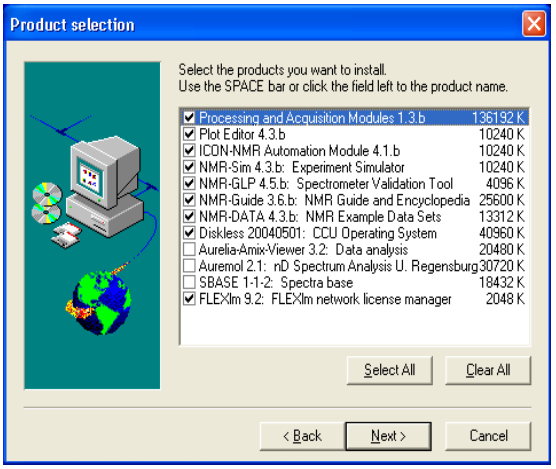
- Click **Next**

8. A window *Select the setup type* will appear:


Select the setup type
Only customized setup allows you to select program components.
Data Processing only
Data Processing, Acquisition and Automation
Customized setup (allows component selection)
< Back
Next >
Cancel

a) Select the setup type. Do one of the following:

- Select *Data Processing, Acquisition and Automation* if you want to use TOPSPIN for spectrometer control. This will install **Diskless** automatically.
- Select *Data Processing* if you want to use TOPSPIN for data processing.
- *Customized setup* (allows components selection) if you want to install selected programs only. If you have selected the following window will appear:


Product selection
Select the products you want to install.
Use the SPACE bar or click the field left to the product name.
Processing and Acquisition Modules 1.3.b 136192 K
Plot Editor 4.3.b 10240 K
ICON-NMR Automation Module 4.1.b 10240 K
NMR-Sim 4.3.b: Experiment Simulator 10240 K
NMR-GLP 4.5.b: Spectrometer Validation Tool 4096 K
NMR-Guide 3.6.b: NMR Guide and Encyclopedia 25600 K
NMR-DATA 4.3.b: NMR Example Data Sets 13312 K
Diskless 20040501: CCU Operating System 40960 K
Aurelia-Amix-Viewer 3.2: Data analysis 20480 K
Auremol 2.1: nD Spectrum Analysis U. Regensburg 30720 K
SBASE 1-1-2: Spectra base 18432 K
FLEXlm 9.2: FLEXlm network license manager 2048 K
Select All
Clear All
< Back
Next >
Cancel

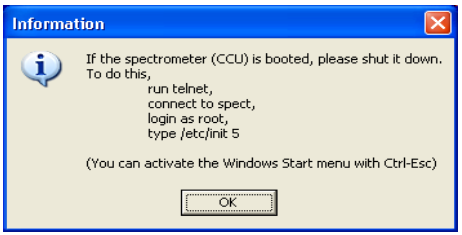
Select the packages which you want to install (note that DISKLESS is only

required if your PC controls a spectrometer or you want to configure it like this.

- ***TOPSPIN***: Acquisition and processing software
- TOPSPIN PLOT EDITOR: Object oriented WYSIWYG plot editor
- ICON-NMR: Icon-driven interface for Routine Spectroscopy and Automation
- DISKLESS: Spectrometer CCU operating system
- NMR-SIM: Program for numerical simulation of NMR experiments
- NMR-GUIDE: web-browser based teaching and training program
- NMR-Data: spectroscopic example data
- AURELIA-AMIX-Viewer: Viewer of 2D/3D/4D NMR data (requires separate license)
- NMR-GLP: Program for 'Good Laboratory Practice' tests (requires separate license)

b) Click **Next**

9. If the *Data Processing, Acquisition and Automation* was selected in step 8, a window *Information* will appear:



If the PC is not yet connected to a spectrometer or if the CCU is not booted[1] you can promptly

- Click **OK**

If your PC is currently connected to a spectrometer and the CCU is booted:

a) Press the keys **CTRL+ESC** (to open the Start menu)

b) Click **Start** → **All Programs** → **Accessories** → **Command Prompt**

c) Enter: **`rsh spect -l root /etc/init 5`**

→ this will shut down the CCU

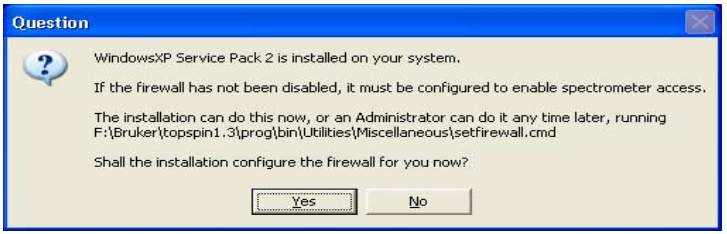
1. Note that during a first time installation of the TOPSPIN the CCU can not be booted.

d) Enter: **`exit`**

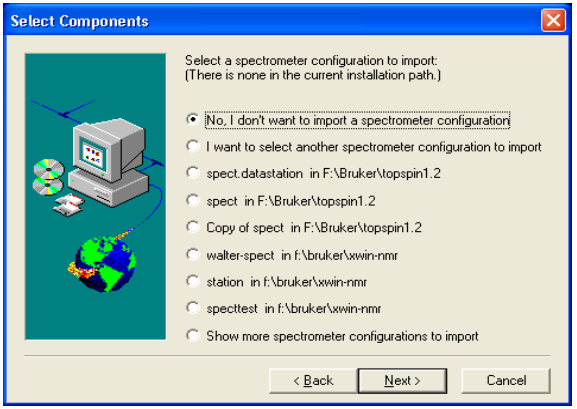
e) Close the window *Information* by clicking **OK**

Note: The CCU is now either down or switched off and should be turned on again at the end of this procedure.

10. A window '*Question*' will appear if Windows XP Service Pack 2 is installed and enabled on your system. If you click ***Yes*** on the installation configure the firewall [1] for you.


Question
WindowsXP Service Pack 2 is installed on your system.
If the firewall has not been disabled, it must be configured to enable spectrometer access.
The installation can do this now, or an Administrator can do it any time later, running F:\Bruker\topspin1.3\prog\bin\Utilities\Miscellaneous\setfirewall.cmd
Shall the installation configure the firewall for you now?
Yes
No

11. A window '*Select Components*' will appear. You can either import no spectrometer configuration, or browse for a spectrometer configuration or select one of the configurations you get offered within this window [2].

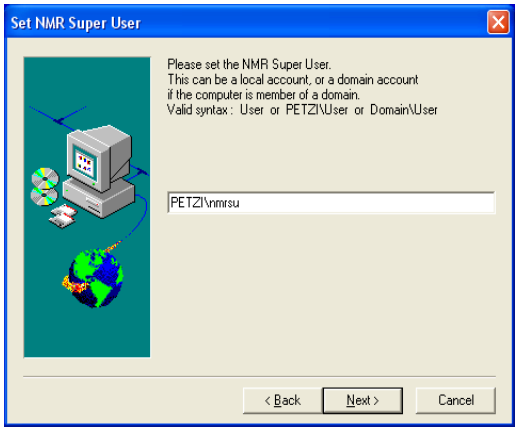

Select Components
Select a spectrometer configuration to import:
(There is none in the current installation path.)
No, I don't want to import a spectrometer configuration
I want to select another spectrometer configuration to import
spect.datastation in F:\Bruker\topspin1.2
spect in F:\Bruker\topspin1.2
Copy of spect in F:\Bruker\topspin1.2
walter-spect in f:\bruker\xwin-nmr
station in f:\bruker\xwin-nmr
specttest in f:\bruker\xwin-nmr
Show more spectrometer configurations to import
< Back
Next >
Cancel

The configurations that are shown in this picture are just an example. On your PC this list could look different.

- Click **Next**

1. The firewall must be configured to enable spectrometer access.
2. The installation process will offer all configurations which are available in the TOPSPIN / XWIN-NMR installation that are defined in the registry.

12. A window '*Set NMR Super User*' will appear:


Set NMR Super User
Please set the NMR Super User.
This can be a local account, or a domain account
if the computer is member of a domain.
Valid syntax : User or PETZI\User or Domain\User
PETZI\nmrsu
< Back
Next >
Cancel

a) Do one of the following:

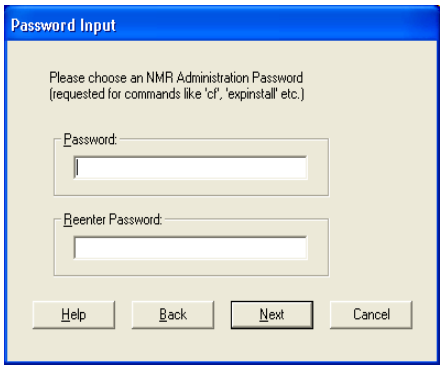
- Accept the default NMR Superuser (Administrator) or
- Enter a special user for this purpose, e.g. named *nmrsu* or
- Enter any other user

Under Windows the username must be the name of an existing user. If you choose an NMR Superuser other than Administrator, and this user does not exist yet:

- Press the keys **CTRL+ESC** (to open the Start menu)
- Install a user as described in chapter 9.

b) Click **Next**

13. A window '*Password Input*' will appear [1] (for more details see chapter 6.2):

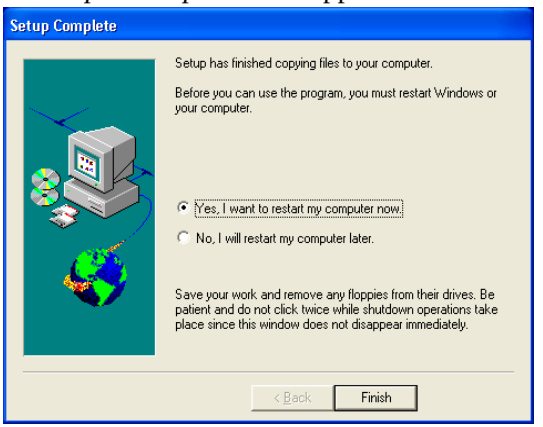


a) Do one of the following:
   - Type in the NMR ADMINISTRATION PASSWORD
   - Re-enter in the NMR ADMINISTRATION PASSWORD

b) Click **Next** → The installation of TOPSPIN will start now.
   - destination directory

c) Click **Next**

14. A window *'Setup is complete'* will appear:


Setup Complete
Setup has finished copying files to your computer.
Before you can use the program, you must restart Windows or your computer.
Yes, I want to restart my computer now.
No, I will restart my computer later.
Save your work and remove any floppies from their drives. Be patient and do not click twice while shutdown operations take place since this window does not disappear immediately.
< Back
Finish

You will be asked if you want to restart the computer:

a) Click **Yes I want to restart my computer now**

b) Click **Finish** (to reboot the computer)

15. After the PC has booted up, press the reset button on the CCU or turn it on with the key if it was switched off. Don't forget to execute '*cf*' and '*expinstall*'.

The following information is for the *Customized setup:*

! • It is strongly recommended to accept the default path for the flexLM installation: '`C:\flexlm`'! If you choose a user defined path, it may cause some problems with other applications using the FlexLM.

1. Certain commands like ***`cf`*** and ***`expinstall`*** ask for the NMR ADMINISTRATION PASSWORD.

6.5 Installing TOPSPIN patches

Bruker BioSpin recommends installing the latest TOPSPIN patches available.

TOPSPIN patches are parts of ***TOPSPIN*** which contain bug fixes. They are available on the Bruker WWW and FTP server. We recommend to install new patches whenever the *patchlevel* on your system is older than the one on the WWW / FTP server.

Perform the following steps:

1. Click on the icon **Bruker Utilities** on the desktop.
2. Click **Miscellaneous** → **Patchlevel**
   This will show you the *patchlevel* on your system.

   Now check if the Patchlevel on the Bruker BioSpin web server is higher than on your system.

Download from WWW server

1. Log in on a computer which is connected to the internet
2. Open your web browser
3. Go to *http://www.bruker-biospin.de*
4. Click on **NMR** → **tech support** → **Software** → **Downloads** → **Linux PC** and select the package you want to download

Download from ftp server

Type **`ftp ftp.bruker.de`**

```
Name: ftp
Password: enter your own full Email address
ftp> cd /pub/nmr/topspin/patches/topspin<vers.>/LINUX
ftp> bin
ftp> ls
```

(if patches are available, you will see a file `topspin-<vers.>-patchX.tar.gz` where X is the patchlevel)

```
ftp> get topspin-<vers.>-patchX.tar.gz
```

```
ftp> get topspin-<vers.>-patchX.readme
ftp> bye
```

Install the patches according to the file `topspin-<vers.>-patchX.readme`

You can also get ***TOPSPIN*** patches from the American FTP server:

ftp.bruker.com:/pub/nmr/mirror.bruker.de/topspin

Check our WWW pages for *known bugs* :

http://www.bruker-biospin.de/NMR/nmrsoftw/passwd/bugs/index.html

6.6 Configuring NFS Server

! If your PC is controlling a spectrometer, you must configure NFS after the installation of the DISKLESS package (part of TOPSPIN). This configuration requires that Hummingbird NFS Server is installed (see chapter 4.3). Once this is installed, you can mount any Windows directory from any UNIX host in your network (see chapter 13.4.4). Basically this chapter finishes the installation started in chapter 4.3.

For this configuration it is very important to turn the Simple File Sharing off:

1. Double-click **My Computer** on the desktop.
2. Click on **Tools**, select **Folder Options**.
3. Click the **View** tab, and then click to select the **Use Simple File Sharing (recommended)** check box to enable Simple File Sharing (click to clear this check box to disable this feature).

1. Click **Start** → **All Programs** → **Accessories** → **Windows Explorer**
2. Select the directory **<TOPSPINHOME>\Diskless** and click with right mouse button.
3. Select in the upcoming window the entry **Properties**
4. Choose the folder **Security**
5. You should see **Full Control** permissions for **Everyone**. Correct this if necessary in the following way:
   - Click **Add**
   - A window *Select Users, Computers, or Groups* will pop up
   - choose the entry **Everyone** in the list **Names**

- Click **Add**
- Click **OK**
- Enable in the '*Permissions*' column '*Allow*' **Full Control**
- Click **OK**
- In most cases especially if your PC controls a spectrometer some error messages could appear. A question if you really want do change the permissions in all the subdirectories of *Diskless* may also occur. You can click ***OK*** in all these windows

6.6.1 Configuring NFS Server 7.1

If you have NFS Server 7.1, proceed as follows:

1. Create the user

- '**diskless_user_sys**' (with '*account is disabled*') [1]

and the groups (with no members)

- '**diskless_group_root**'
- '**diskless_group_other**'
- '**diskless_group_sys**'

2. Click **Start** → **Control Panel**

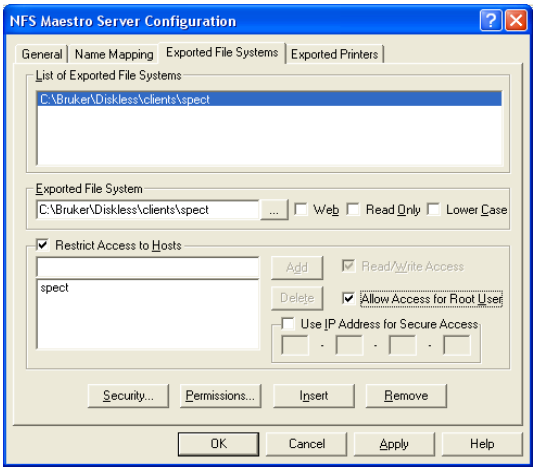
3. The window '*Control Panel*' will appear:

- Double-click the icon **Hummingbird NFS Server**

4. A window '*NFS Maestro Server*' will appear:

1. Creation and configuration of the necessary user and groups are most convenient if it is done in the user management tool of the management console and not in the user management of the control panel. For starting the management console click right on 'My computer' and choose 'manage'. A new window appears where you can choose 'local users and groups'

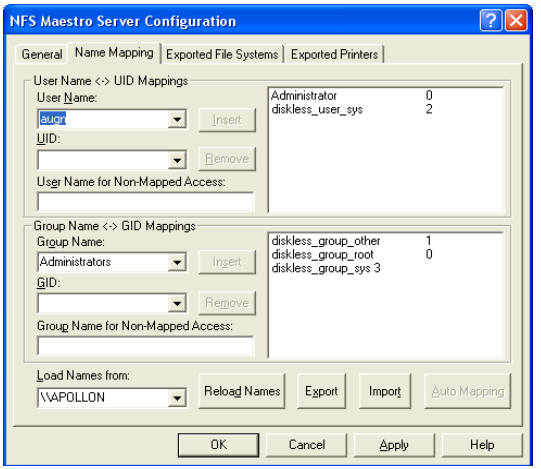
a) Click the **Exported File Systems** tab



- In the field **Exported File System**: browse for the location of the DISKLESS package (e.g.: `C:\Bruker\Diskless\clients\spect`)

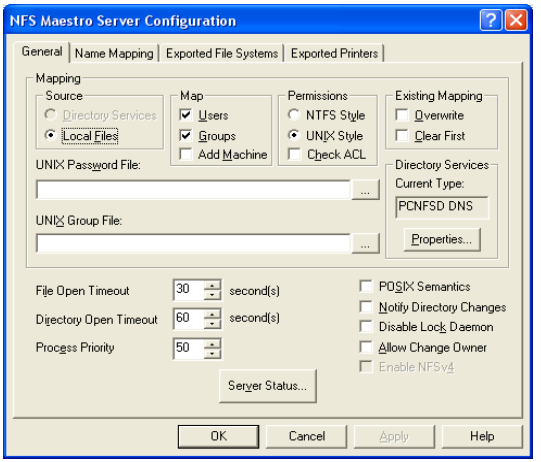
  Important: the Uppercase letters in this path are necessary!
- Select the **Allow Access for Root User**
- Select **Restrict Access to Hosts**, enter **spect** in the field below and click **Add** → the name spect will appear in the list '*Restricted Access to Hosts*'
- Click **Insert** → 'spect' appears in 'Lists of Exported File Systems'

b) Click the **Name Mapping** tab



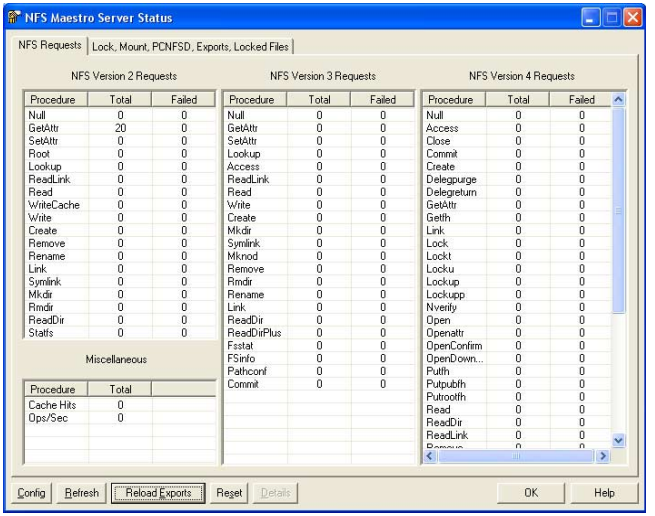
- Click the arrow to the right of the field *Load NT Names from* and select the local hostname, e.g. **MYHOST**
- Click **Reload Names**
- Adding a User mapping
  - In the field *User Name* select the user **Administrator**
    - In the field below, that is called '*UID*' type in '**0**'
    - Click **Insert**
  - In the field *User Name* select **diskless_user_sys**.
    - In the field below, that is called '*UID*' type in '**2**'
    - Click **Insert**
- Adding a Group mapping
  - Select the Group Name using the arrow button in the field below it, type in the GID and click **Insert**
    - Map the group **diskless_group_root** as group with GID 0
    - Map the group **diskless_group_other** as group with GID 1
    - Map the group **diskless_group_sys** as group with GID 3

c) Click the **General** tab



- Click **Server Status**

d) A window '*NFS Maestro Server Status*' will appear:



- Click **Reload Exports**
- Click **OK**

5. In the window '*NFS Maestro Server Configuration*' → Click **OK**

6. If a message about the owner and permissions of spect appears:

- Click **Yes**
- A window '*Permissions*' will appear:
  - Select User: '*Administrator*' and enable Read, Write and Execute permissions for this user
  - Select Group: '*diskless_group_root*' and enable Read, Write and Execute permissions for this group
  - Be sure that also '*other*' has Read, Write and Execute permissions
  - Click **Recursive** → Click **OK**

7. Close the window '*Control Panel*' by clicking the **X** button.

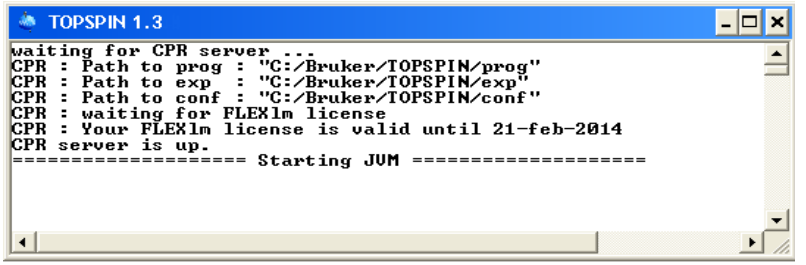
6.7 Adding a user to the group NmrUser

! Every user who wants to run TOPSPIN must be member of the group NmrUser. Adding users to this group is described in chapter 9.1.3.

6.8 Check if the TOPSPIN installation is correct

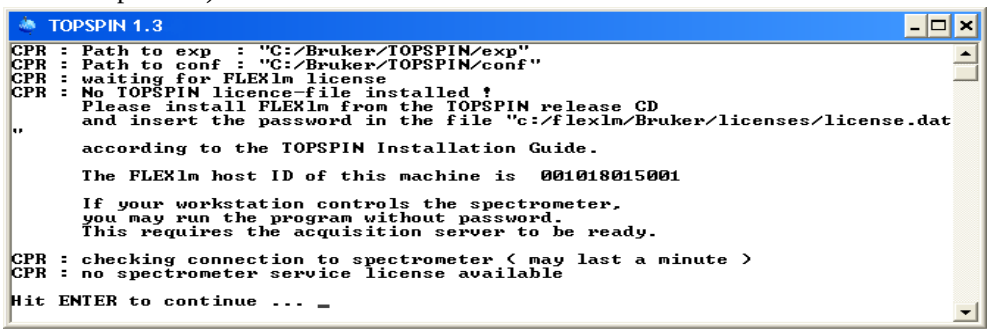
Double click the TOPSPIN-icon

If you have an valid license you will get this screen.


TOPSPIN 1.3
waiting for CPR server ...
CPR : Path to prog : "C:/Bruker/TOPSPIN/prog"
CPR : Path to exp : "C:/Bruker/TOPSPIN/exp"
CPR : Path to conf : "C:/Bruker/TOPSPIN/conf"
CPR : waiting for FLEXlm license
CPR : Your FLEXlm license is valid until 21-feb-2014
CPR server is up.
==================== Starting JVM ====================

and Topspin will start.

Unless you already have a license you will get this screen (for further details see chapter 7.2)::


TOPSPIN 1.3
CPR : Path to exp : "C:/Bruker/TOPSPIN/exp"
CPR : Path to conf : "C:/Bruker/TOPSPIN/conf"
CPR : waiting for FLEXlm license
CPR : No TOPSPIN licence-file installed !
Please install FLEXlm from the TOPSPIN release CD
and insert the password in the file "c:/flexlm/Bruker/licenses/license.dat
"
according to the TOPSPIN Installation Guide.
The FLEXlm host ID of this machine is 001018015001
If your workstation controls the spectrometer,
you may run the program without password.
This requires the acquisition server to be ready.
CPR : checking connection to spectrometer (may last a minute)
CPR : no spectrometer service license available
Hit ENTER to continue ...

6.9 Compiling AU programs

TOPSPIN only needs a compiler for the compilation of AU programs. If you do not use AU programs, you do not need a compiler!

TOPSPIN is delivered with the free GNU *gcc* compiler.[1]

It is installed automatically during installation of TOPSPIN.

6.10 The usage of the NMR-GUIDE

NMR-GUIDE 4.0 that comes with TOPSPIN 1.3 uses an own web server and the TOPSPIN internal java package. Therefore it is not necessary anymore to have these packages installed/configured separately!

6.10.1 Requirements for NMR Guide 4.0

The using of NMR-GUIDE 4.0 requires the installation of TOPSPIN 1.3. Also be sure that the following components are installed:

1. Web browser *Microsoft Internet Explorer*
2. *PDF viewer*

   NMR-GUIDE offers among other things a lot of PDF documents. To display these documents it is necessary to install the acrobat reader. For an installation description see chapter 5.1
3. NMR-GUIDE license (contact license@bruker.de for a three month demo license or order a official license from your local Bruker representative). Note that the NMR-GUIDE license is already part of a full or demo ***TOPSPIN*** 1.3 license.

The *Microsoft Internet Explorer* is an official part of the operating system *Microsoft Windows XP*. The WWW browser gets documents from the locally installed WWW server. The client - server communication is established over a network socket connection, but the communication partners only use the localhost TCP/IP host identifier. These pages are shown in the right-hand side window of the browser.

The WWW browser also gets dynamically created pages from the localhost. These workstation specific pages are coming from a *gserver*. This is a platform independent Java web server written by Bruker BioSpin and acts as a daemon running on the locally installed JAVA virtual machine. The gserver is included in the NMR Guide&Encyclopedia package. The table of contents is generated dynamically and displayed in the left-hand side window of the browser.

`TOPSPIN` commands can be invoked from the WWW browser. This process is also managed by the gserver. The gserver is an essential component of the NMR Guide&Encyclopedia and requires an NMR-GUIDE license.

1. If you like to work with the '*vi*' in Bruker's GNU shell, it is necessary to start it with the command '*vim*' in this version of the GNU package.

6.10.2 Java Requirements for NMR-GUIDE 4.0

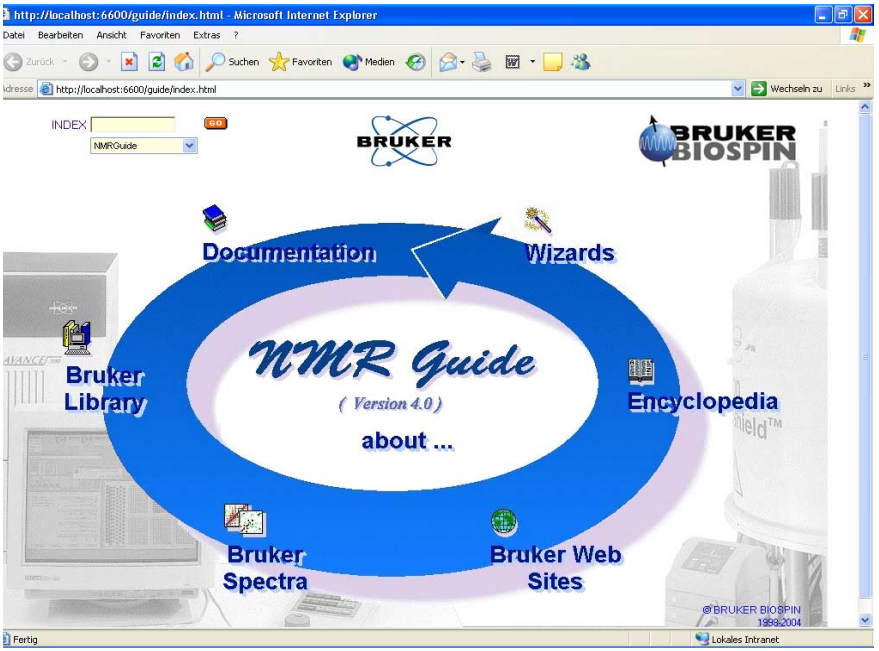
For using NMR-GUIDE 4.0 that comes with the TopSpin 1.3 version it is not necessary to install/configure a special Java package. NMR-GUIDE uses the TopSpin internal Java package that is automatically installed and configured during installation of TopSpin.

6.10.3 Working with the NMR-GUIDE

In order to work with the NMR-GUIDE, the following procedure must be followed.

- Start up of the NMR-GUIDE
  1. Start TOPSPIN and enter the command: ***ghelp***
  2. or enter the command (this allows to start a search within NMR-GUIDE: ***help***
  3. or select from the ***Help*** pull-down menu of TOPSPIN the entry: ***NMR-GUIDE***

  Your standard web browser will automatically starts and shows the page:



6.10.4 Configuration of Internet Explorer for the NMR-GUIDE

1. Click **Start** → **All Programs** → **Internet Explorer**
2. A window *Microsoft Internet Explorer* will appear
3. Click on **Tools** → **Internet Options** → **Advanced**
4. Ensure that the following Settings are enabled:
   - Java console enabled (requires restart)
   - Java logging enabled
   - JIT compiler for virtual machine enabled (requires restart)
5. Restart your computer

Chapter 7

The TOPSPIN license

7.1 Questions and answers about the TOPSPIN license

1. *Which programs need a license?*

TOPSPIN, TOPSPIN PLOT EDITOR, NMR-SIM and NMR-GUIDE need a license. However, if you order a license for TOPSPIN, you automatically get a license for all four programs.

If you do not have a license for TOPSPIN, it will start up in an emergency mode if your PC is connected to a spectrometer. However, NMR-SIM and NMR-GUIDE will not run without a valid license.

ICON-NMR is always used in connection with TOPSPIN and does not need an individual license.

AURELIA, AMIX, MAXENT, GLP and PARAVISION do need a license which must be ordered for each program separately.

2. *Which license types are available and what programs may be run with each?*

There are six different license types, details of each are given in the following table. For more information please refer to the Bruker license order form in the help menu of TOPSPIN or on the web server:

`http://www.bruker-biospin.de/NMR/nmr-softw/passwd/docu/index.html`

or contact your local Bruker BioSpin representative.

License type	Contents
Full	Acquisition, Processing, Automation (ICON-NMR), Plotting, Experiment Simulation and NMR-GUIDE
	license period: 15 years
	no restrictions
Additional	Acquisition, Processing, Automation (ICON-NMR), Plotting, Experiment Simulation and NMR-GUIDE
	license period: 15 years
	one Full license has to be available
Demo	Acquisition, Processing, Automation (ICON-NMR), Plotting, Simulation and NMR-GUIDE
	license period: 3 months
	Node locked, uncounted, free of charge
Processing-Only	Processing and Plotting
	license period: 15 years
	no Acquisition, no NMR-SIM, no NMR-GUIDE
Presenter	Viewing and Plotting
	license period: 15 years
	no Processing, no NMR-SIM, no NMR-GUIDE
Teaching	NMR-SIM and restricted Processing and Plotting
	license period: 15 years
	TopSpin can only process datasets that are older than 4 weeks or datasets created by NMR-SIM. One TopSpin-plot session (without portfolio editor) can be started, Node locked, count 1.
Developer	Special license for extending TOPSPIN with own functionalities. Allows viewing of data.
	license period: unlimited
	no Processing, no Plotting, no NMR-SIM, no NMR-GUIDE, free of charge

3. *What kind of licenses do I need?*

If you want to use TOPSPIN 1.x you need a FEATURE line '*TOPSPIN1*' in your `license.dat` file. If you have '*XWINNMR3*' you can only start XWIN-NMR

3.x.

If more than one license is available, as many copies of the program as are covered by the license can be started simultaneously.

4. *Which licensing program is used for TOPSPIN?*

The Flexlm license manager is used and is delivered on the TOPSPIN CDROM. The Flexlm package occupies about 3 MByte of disk space. It contains the *'lmgr'* license manager, the *'lmutil'* program, Help files and example `license.dat` file.

5. *What are the requirements for the Flexlm to function:*

- your PC must have an Ethernet card
- the network (TCP/IP) must be installed
- the network Service *'NetBIOS Interface'* must be installed

6. *What is a Floating license?*

Floating licenses are licenses that are available for more than one computer in a network. *Floating* licenses are issued based on the Host-ID of one particular computer. This computer becomes the "license server". All computers that can communicate with this "license server" computer can use the licenses managed by this computer. For this to work, the same license file must be installed on all participating computers, including the "license server". The Flexlm license manager software must only run on the "license server" computer.

A *Floating* license can have just one license for a program like TOPSPIN. In such a case, the respective program can be started once on one computer in the network. If more than one license is available, as many copies of the program as are covered by the license can be started simultaneously. For example, if you have a license file with 5 licenses for TOPSPIN, TOPSPIN can be started 5 times from any 5 computers in the network.

The number of licenses is stated in the FEATURE for the respective program.

7. *What is the difference between 1-Server / 3-Server Licenses?*

Floating licenses can be ordered as 1-server or 3-server licenses. In a 1-server license you have only one license server, and in a 3-server license there are three license servers defined in the license file.

- The advantage of a 1-server license is that it is only necessary to have one computer active at a time to make the license available.

- The advantage of a 3-server license is that any of the three license servers can be inactive and the license management is then done by the remaining two servers.
- One requirement for the three license servers is that all of them have TCP/IP active.
- The operating system on the three computers can be the same or can be different (Linux, Windows).

8. *What is a Node Locked license?*

A node-locked license allows you to start the respective program only on the computer with the Host-ID for which that license was generated. Typically, this license form is used for Demo and Teaching licenses. No other computer can use the license in the way described above for floating licenses.

9. *How do I know if my license is* Floating *or* Node Locked*?*

You can recognize this from the syntax of the license FEATURES in the `license.dat` file:

on PC:

`c:\flexlm\bruker\licenses/license.dat`

on Linux:

`/usr/local/flexlm/Bruker/licenses/license.dat`

If the entry *'HOSTID='* appears after the encrypted password, the license is Node locked and can only be used on the local PC.

FEATURE TOPSPIN1 bruker_ls 0.0 6-aug-2018 3 \
9B1EA0113CD53A883974 HOSTID=006008d244fe vendor_info=....

→ *Node locked* license for three parallel sessions of TOPSPIN that can be started on the local PC

FEATURE TOPSPIN1 bruker_ls 0.0 6-aug-2018 3 9B1EA0113CD53A883974 vendor_info=....

→ *Floating* license for three parallel sessions of TOPSPIN that can be started on every PC in the local network

10. *If I have a* Floating *license and I have a dual-boot PC (e.g Windows XP and Linux), can I use the license on both operating systems?*

Yes, the license is based on the physical address of the Ethernet card and not on the operating system. Copy the license file `license.dat` to:

Windows:

```
c:\flexlm\Bruker\licenses\license.dat
```

Linux:

```
/usr/local/flexlm/Bruker/licenses/license.dat
```

11. *How can I determine the hostid of my PC?*

See chapter 7.2.1.

12. *How do I install a license (full or demo) on my PC?*

See chapter 7.2.

13. *Does a Demo license require SERVER/DAEMON lines in* `license.dat`*?*

No, a Demo license is *Node Locked* and therefore only requires FEATURE lines. If SERVER and/or DAEMON lines exist, they are ignored.

14. *I have a* Floating *license. Must the file* `license.dat` *be identical on all hosts, server and clients?*

Yes, you can install `license.dat` on the server and then copy it to all clients.

15. Must the Flexlm license manager run on all hosts in the network?

No, it only needs to run on the license server. If the license manager also runs on a license client, this is simply ignored.

16. *Must the Flexlm license manager run on a host with a Demo license?*

No, it only needs to run on the server for *Counted* licenses.

17. *What can I do if TOPSPIN does not start after I installed the license?*
See chapter 15 .

18. *How is it possible that TOPSPIN starts even though I do not have a license?*

If you do not have a license for TOPSPIN, it will start up in an emergency mode if your PC is connected to a spectrometer. Also one TOPSPIN PLOT EDITOR session (without portfolio editor) can be started from within TOPSPIN. However, NMR-SIM and NMR-GUIDE will not run without a valid license.

19. *What can I do if TOPSPIN cannot find the license server?*

Please try to restart the license server:

1. Open the Management Console:
   My Computer -> right click **Manage**
2. A window will appear:

Right click Bruker FLEXlm License Server -> right click **Properties**

3. A window will appear:
   If the Service status is 'Started' click *Stop* -> wait and then click *Start* again
   If the Service status is 'Stopped' click *Start*

7.2 Ordering and installing the TOPSPIN license

You can order a license from Bruker BioSpin Germany. Demo licenses are free of charge, for other licenses you must specify:

- the hostid of your PC (see chapter 7.2.1)
- the program for which you want to get a license, e.g. TOPSPIN
- the type of license (full, demo, processing-only, presentation or teaching)
- the number of licenses and your order number (not necessary for demo license)

Licenses can be ordered from the German Bruker BioSpin web server:

https://www.bruker-biospin.de/NMR/nmrsoftw/licenses/index.html

7.2.1 How do I determine the correct hostid

The hostid is a 12-digit hexadecimal number. It is the physical address (also called Mac address or Node address) of the Ethernet card. After installing TOPSPIN, including the Flexlm license manager, you can determine the hostid in two ways:

- Start TOPSPIN; a command prompt will pop up, which will list the hostid, if a correct licence is not yet installed.
- Click the **Bruker Utilities** icon on the desktop, then click **Miscellaneous** → **get_hostid**
- Open a Command Prompt and type in:
  `c:\flexlm\bruker\lmutil lmhostid`

  Under Windows XP it is possible to get more than one hostid. Just select one of them to order the license.

Some hostid values may indicate problems:

a) If hostid '*2*' occurs: You may run Windows XP and your network-adapters are disabled.
   Click **Start** → **Control Panel** → **Network Connections**

Right-click all **Local Area Connection xxx -**items and there
click **Enable** (if it is visible)

b) If hostid *'0'* or *'ffffffff'* occurs: You may run Windows XP and your network-adapter has no link to the network.

Establish an link to the network or install the

`NWlink IPX/SPX/NetBIOS Compatible Transport Protocol:`
Click **Start** → **Control Panel** → **Network Connections**
Right-click **Local Area Connection xxx**

Click **Properties** → **Install...** → **Protocol** → **Add**
The *`Select Network Protocol`*-menu will appear after some seconds.
Click **NWlink ...** → **OK**
After some seconds the Properties-menu will reappear: Click **Close**
See also

`C:\flexlm\Bruker\help\Index.htm`

for FlexLM-related problems

7.2.2 Installing a Demo license

A Demo license can be installed as follows:

1. Log in as Administrator
2. Install the Flexlm license manager as described in chapter 6.4.
3. Open a Command Prompt and enter:
   - **`cd /d c:\flexlm\Bruker\licenses`**
   - **`notepad license.dat`**

     enter the FEATURE lines, save and exit the file

You can also install the license file from the Explorer. We have chosen the Command Prompt because the Explorer might add the (perhaps hidden) extension `.txt` to the file `license.dat` which makes it unusable (see chapter 16.1.3).

7.2.3 Installing a full license on a license server

The Flexlm license manager must always be installed and run as an Windows XP service on the license server. It is delivered on the TOPSPIN CDROM and can be installed as described in chapter 6.4. The Flexlm is automatically installed as a

Windows XP Service which is then automatically started.

On the license server, the file license.dat must contain a SERVER line, a DAEMON line and FEATURE lines. An example would be:

```
SERVER tulip 0060080e830d 1700
DAEMON bruker_ls c:\flexlm\Bruker\bruker_ls.exe
FEATURE TOPSPIN1 bruker_ls 0.0 6-aug-2018 3 0B0E4011FF0CD32FBFF1 \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE TOPSPIN_1D bruker_ls 0.0 6-aug-2018 3 9B3EA021818829E2716A \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE TOPSPIN_2D bruker_ls 0.0 6-aug-2018 3 AB3E80014D54F0FB3887 \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE XWINPLOT bruker_ls 0.0 6-aug-2018 3 DB4E50F1618A2B2383D3 \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE TOPSPIN_ACQU bruker_ls 0.0 6-aug-2018 3 9BDE3051D4CB63255DCC \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
FEATURE NMRSIM bruker_ls 0.0 6-aug-2018 3 2B4EC041E98523510FCB \
vendor_info=" for hostid(s) : 0060080e830d" ISSUER=00047573d35e
```

where *tulip* is the hostname and *0060080e830d* the hostid of the computer. Note that the second part of the FEATURE lines, the vendor_info, does not necessarily exist. In that case a FEATURE line would look like:

```
FEATURE TOPSPIN1 bruker_ls 0.0 6-aug-2018 3 0B0E4011FF0CD32FBFF1""
```

To inform Flexlm about the new license proceed as follows:

1. Open the **Windows Explorer** and go to `<Flexlm_Home>\Bruker\` → Double-click `lmtools.exe`
2. A window '*LMTOOLS*' appears. Click the **Start/Stop/Reread** tab → Click **Stop Server** → Click **Start Server** → Click **ReRead License file** → Click **OK**
3. Close the window '*LMTOOLS*' by clicking the **X** button.

7.2.4 Installing a full license on a license client

On a license client, license can be installed in two different ways, as described for a Demo license chapter 7.2.2. The only difference is that you do not have to setup a new file `license.dat`. You can just copy it from the license server which can be another PC (see question 10 in chapter 7.1).

7.2.5 Modifying the license file

To inform Flexlm about the new license proceed as follows:

1. Open the **Windows Explorer** and go to `<Flexlm_Home>\Bruker\` → Double-click `lmtools.exe`
2. A window '*LMTOOLS*' appears. Click the **Start/Stop/Reread** tab → Click **Stop Server** → Click **Start Server** → Click **ReRead License file** → Click **OK**
3. Close the window '*LMTOOLS*' by clicking the **X** button.

7.2.6 Further information

For more information on the Flexlm license manager:

Click **Start** → **run** enter **`c:\flexlm\bruker\help\index.htm`** click **OK**

If TOPSPIN does not start after installing the license, please check chapter 15.

Chapter 8

Configuration of TOPSPIN

The idea of this chapter is to give you some guidelines to full spectrometer or workstation configuration. We do not discuss the commands in detail here. For a full description refer to the TOPSPIN manual.

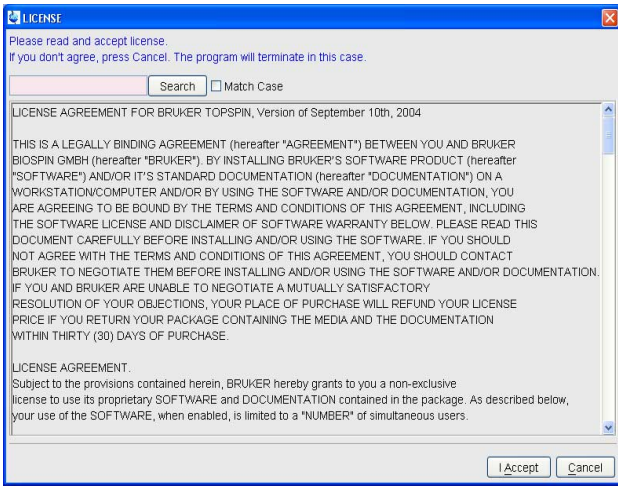
8.1 Configuring TOPSPIN

There are two ways to start TOPSPIN:

1. Click the icon TOPSPIN on the desktop

2. Click **Start** → **All Programs** → **Bruker TOPSPIN** → **TOPSPIN<vers.>**

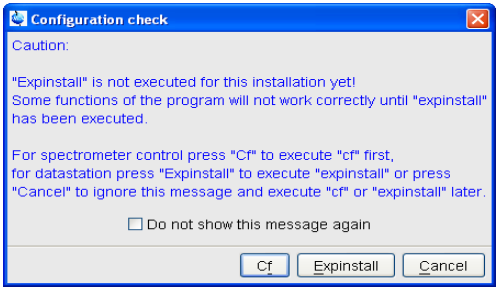
After the first startup of TOPSPIN a window 'License' will appear:


LICENSE
Please read and accept license.
If you don't agree, press Cancel. The program will terminate in this case.
Search
Match Case
LICENSE AGREEMENT FOR BRUKER TOPSPIN, Version of September 10th, 2004
THIS IS A LEGALLY BINDING AGREEMENT (hereafter "AGREEMENT") BETWEEN YOU AND BRUKER BIOSPIN GMBH (hereafter "BRUKER"). BY INSTALLING BRUKER'S SOFTWARE PRODUCT (hereafter "SOFTWARE") AND/OR IT'S STANDARD DOCUMENTATION (hereafter "DOCUMENTATION") ON A WORKSTATION/COMPUTER AND/OR BY USING THE SOFTWARE AND/OR DOCUMENTATION, YOU ARE AGREEING TO BE BOUND BY THE TERMS AND CONDITIONS OF THIS AGREEMENT, INCLUDING THE SOFTWARE LICENSE AND DISCLAIMER OF SOFTWARE WARRANTY BELOW. PLEASE READ THIS DOCUMENT CAREFULLY BEFORE INSTALLING AND/OR USING THE SOFTWARE. IF YOU SHOULD NOT AGREE WITH THE TERMS AND CONDITIONS OF THIS AGREEMENT, YOU SHOULD CONTACT BRUKER TO NEGOTIATE THEM BEFORE INSTALLING AND/OR USING THE SOFTWARE AND/OR DOCUMENTATION. IF YOU AND BRUKER ARE UNABLE TO NEGOTIATE A MUTUALLY SATISFACTORY RESOLUTION OF YOUR OBJECTIONS, YOUR PLACE OF PURCHASE WILL REFUND YOUR LICENSE PRICE IF YOU RETURN YOUR PACKAGE CONTAINING THE MEDIA AND THE DOCUMENTATION WITHIN THIRTY (30) DAYS OF PURCHASE.
LICENSE AGREEMENT.
Subject to the provisions contained herein, BRUKER hereby grants to you a non-exclusive license to use its proprietary SOFTWARE and DOCUMENTATION contained in the package. As described below, your use of the SOFTWARE, when enabled, is limited to a "NUMBER" of simultaneous users.
I Accept
Cancel

a) Please read the License Agreement for TOPSPIN!

b) When you have finished reading the License Agreement for TOPSPIN and you can confirm the agreement click on **I accept**.

After the window 'License' a window 'configuration check' appears:


Configuration check
Caution:
"Expinstall" is not executed for this installation yet!
Some functions of the program will not work correctly until "expinstall" has been executed.
For spectrometer control press "Cf" to execute "cf" first,
for datastation press "Expinstall" to execute "expinstall" or press
"Cancel" to ignore this message and execute "cf" or "expinstall" later.
Do not show this message again
Cf
Expinstall
Cancel

Please configure the software (depends on the hardware of your spectrometer). If you do this, you are mainly in one of the four following situations:

- You have just installed the software in a new directory and the old spectrometer configuration of the software is still known to the new version → go to chapter 8.1.1
- You want to configure a only-processing-PC like your spectrometer-PC, so you have the spectrometer configuration on another computer → go to chapter 8.1.2

- You have to configure the software on a new hard disk without a backup of the spectrometer configuration, so you have no configuration files anymore → go to chapter 8.1.4
- You have a new spectrometer hardware component, so you have no configuration file so far → go to chapter 8.1.5

If you would like to take over the configuration of an existing XWIN-NMR/TOPSPIN into TOPSPIN 1.3 please check chapter 8.2.

8.1.1 If your PC controls a spectrometer:

1. Be sure that the spectrometer is booted (see chapter 6.4 and 15.5.3)

2. Open a dataset

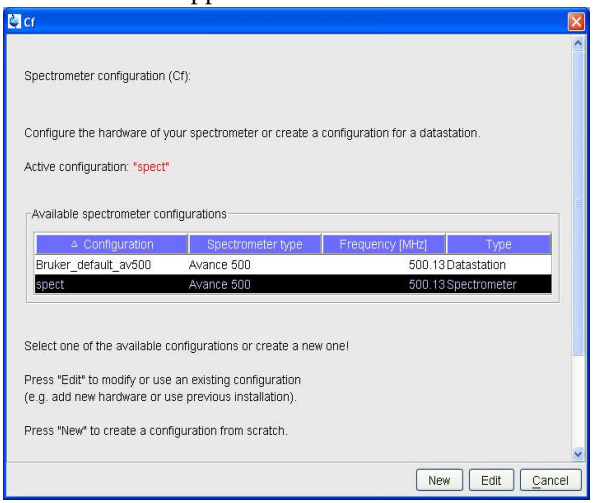
- Type ***new*** and create a new dataset.
- You can also select a dataset (e.g. *exam1d_1h*) acquired with another TOPSPIN or XWIN-NMR version.

3. Enter ***cf*** (The command ***cf*** now configures the software according to the hardware of your spectrometer):

a) A window will appear:
Password request. Please enter the NMR administration password

Type in the NMR ADMINISTRATION PASSWORD. Click **OK**.

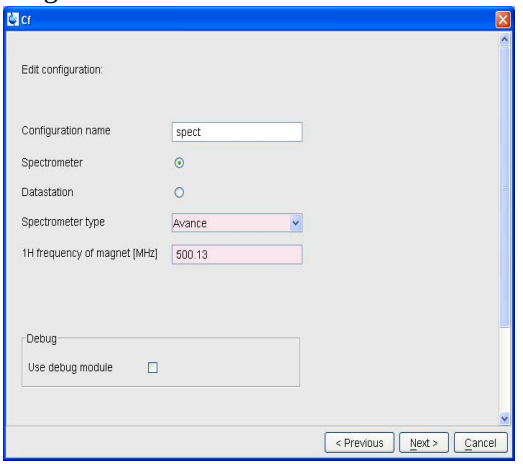
b) A window will appear:.



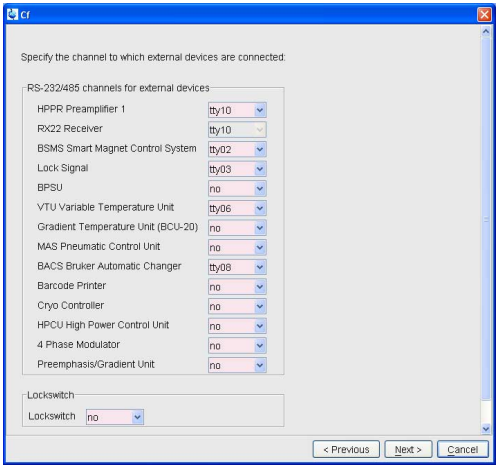
Most likely you will select an existing configuration and press "Edit" to confirm this configuration.

c) A window will appear:

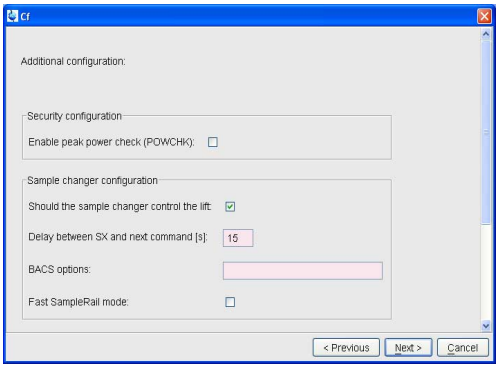
The selected configuration is displayed. Choose if would to configure it as a spectrometer or datastation. Choose the type of your spectrometer e.g. ***AVANCE*** → **ENTER**. Check or type in the 1H frequency of the magnet e. g. ***500.13*** → **ENTER**. Use the debug mode only in a case of trouble-shooting.



d) A window will appear:
Check if the tty-numbers of the hardware components are set correctly..



- A window for additional configuration will appear:



- Choose the option if you need this security options.

  Enable peak power check (POWCHK): (yes/no)

- If you have a sample changer, please select:

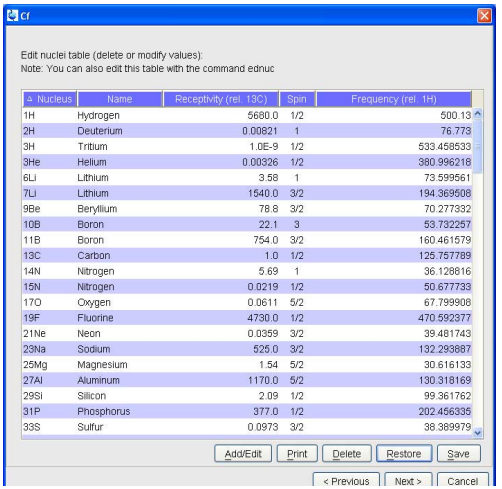
  Should the Sample Changer control the Lift: (yes/no)

  The answer depends on how the air flow is connected, normally you will answer: ***yes***

  Delay between SX and next command [sec]?

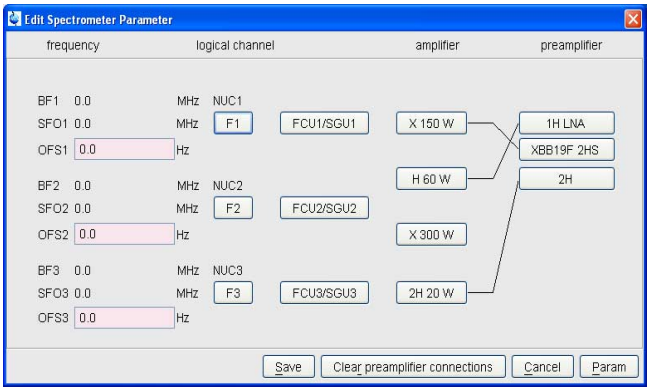
  Type in the length of the delay e. g. ***10*** → **ENTER**

e) The *nuclei-table* appear.

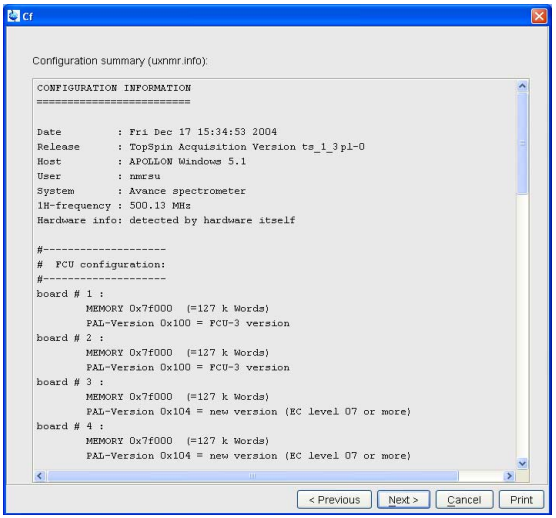

Cf
Edit nuclei table (delete or modify values):
Note: You can also edit this table with the command ednuc
Nucleus Name Receptivity (rel. 13C) Spin Frequency (rel. 1H)
1H Hydrogen 5680.0 1/2 500.13
2H Deuterium 0.00821 1 76.773
3H Tritium 1.0E-9 1/2 533.458533
3He Helium 0.00326 1/2 380.996218
6Li Lithium 3.58 1 73.599561
7Li Lithium 1540.0 3/2 194.369508
9Be Beryllium 78.8 3/2 70.277332
10B Boron 22.1 3 53.732257
11B Boron 754.0 3/2 160.461579
13C Carbon 1.0 1/2 125.757789
14N Nitrogen 5.69 1 36.128816
15N Nitrogen 0.0219 1/2 50.677733
17O Oxygen 0.0611 5/2 67.799908
19F Fluorine 4730.0 1/2 470.592377
21Ne Neon 0.0359 3/2 39.481743
23Na Sodium 525.0 3/2 132.293887
25Mg Magnesium 1.54 5/2 30.616133
27Al Aluminum 1170.0 5/2 130.318169
29Si Silicon 2.09 1/2 99.361762
31P Phosphorus 377.0 1/2 202.456335
33S Sulfur 0.0973 3/2 38.389979
Add/Edit
Print
Delete
Restore
Save
< Previous
Next >
Cancel

Check if the frequency of the nuclei are set correctly and click ***Save*** (If in doubt click ***Restore*** then click ***Save***)

f) A window 'Edit spectrometer configuration will appear:
Check if the preamplifier connections are set correctly and click ***Save***..

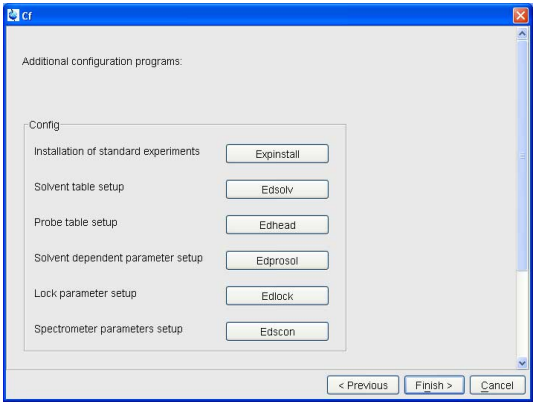


g) The results of ***cf*** appears in a text window. Check this list carefully and compare the result with an list from an earlier configuration (if available) click ***Print*** and store the paper output with your other spectrometer documentation, then click ***Next.***.


cf
Configuration summary (uxnmr.info):
CONFIGURATION INFORMATION
Date : Fri Dec 17 15:34:53 2004
Release : TopSpin Acquisition Version ts_1_3 pl-0
Host : APOLLON Windows 5.1
User : nmrsu
System : Avance spectrometer
1H-frequency : 500.13 MHz
Hardware info: detected by hardware itself
board # 1 :
MEMORY 0x7f000 (=127 k Words)
PAL-Version 0x100 = FCU-3 version
board # 2 :
MEMORY 0x7f000 (=127 k Words)
PAL-Version 0x100 = FCU-3 version
board # 3 :
MEMORY 0x7f000 (=127 k Words)
PAL-Version 0x104 = new version (EC level 07 or more)
board # 4 :
MEMORY 0x7f000 (=127 k Words)
PAL-Version 0x104 = new version (EC level 07 or more)
< Previous
Next >
Cancel
Print

If during 'cf' an error message occurs that invites you to do a firmware update see chapter 8.5

After finishing cf window *'Additional configuration programs'* will appear showing a list of configuration steps. .

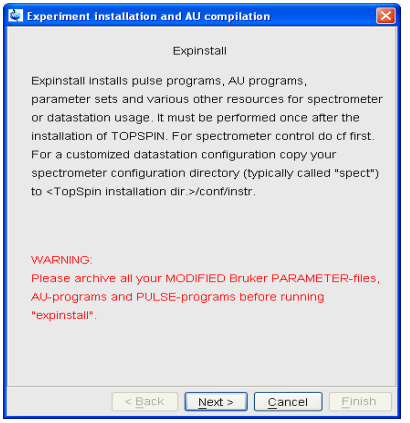


Accept the default selection and click on the buttons (You will be asked for the NMR ADMINISTRATION PASSWORD a couple of times):

- Continue with ***expinstall***

a) Type in the NMR ADMINISTRATION PASSWORD and **OK**

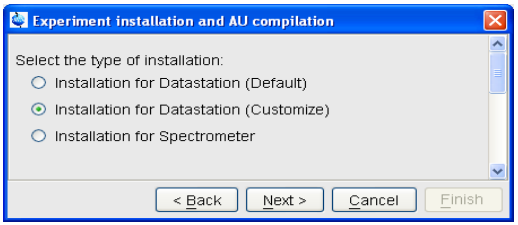
b) Click **Next** if you either have no modified Bruker BioSpin-Parameterfiles


Experiment installation and AU compilation
Expinstall
Expinstall installs pulse programs, AU programs, parameter sets and various other resources for spectrometer or datastation usage. It must be performed once after the installation of TOPSPIN. For spectrometer control do cf first. For a customized datastation configuration copy your spectrometer configuration directory (typically called "spect") to <TopSpin installation dir.>/conf/instr.
WARNING:
Please archive all your MODIFIED Bruker PARAMETER-files, AU-programs and PULSE-programs before running "expinstall".
< Back
Next >
Cancel
Finish

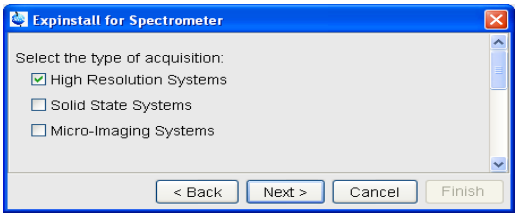
AU-programs and Pulse-programs or if you have archive them in a different

directory. Your individual Parameterfiles, AU-programs and Pulse-programs that have different names to the original Bruker BioSpin files will not be destroyed during the installation

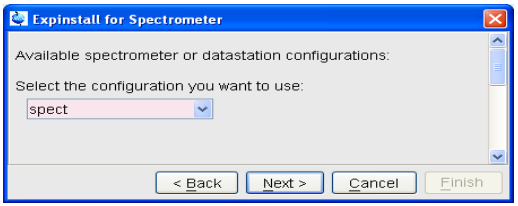
c) In the window that appears → Check *Installation for Spectrometer* → Click ***Next***



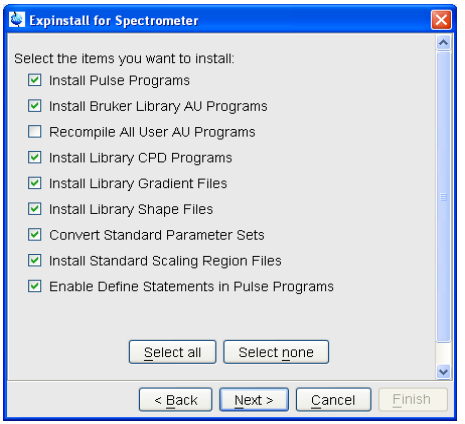
d) In the window that appears → Check *High Resolution Systems* → Click ***Next***



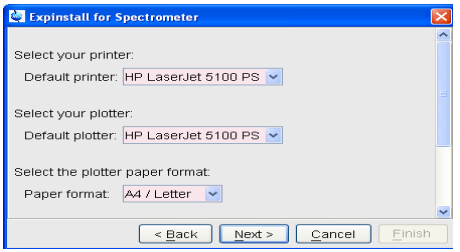
e) In the dialog box that appears → Select the spectrometer configuration name → Click ***Next***



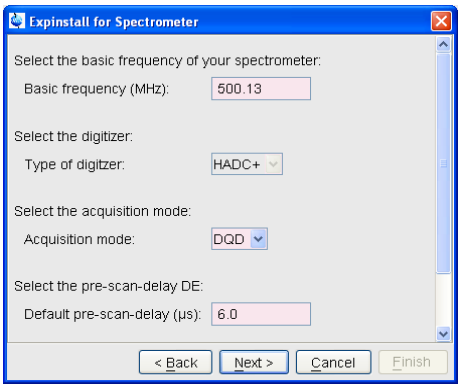
In the dialog box that appears → Check the items you want to install or, accept the default selection → Click ***Next***



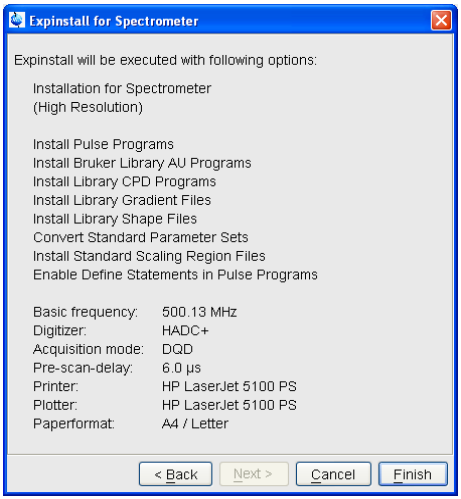
f) In the dialog box that appears → Select the default printer and plotter and the desired paper format → Click ***Next***



g) In the window that appears → Enter the desired spectrometer frequency, acquisition mode and pre-scan-delay or, accept the default values
→ Click ***Next***

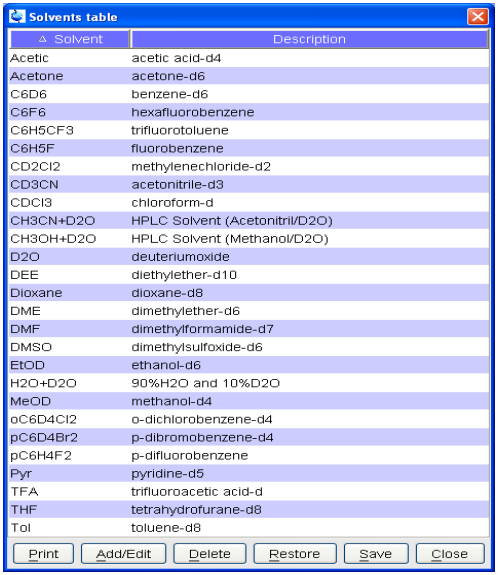


h) In the information box that appears → Check the configuration selection and, if it is correct → Click ***Finish***



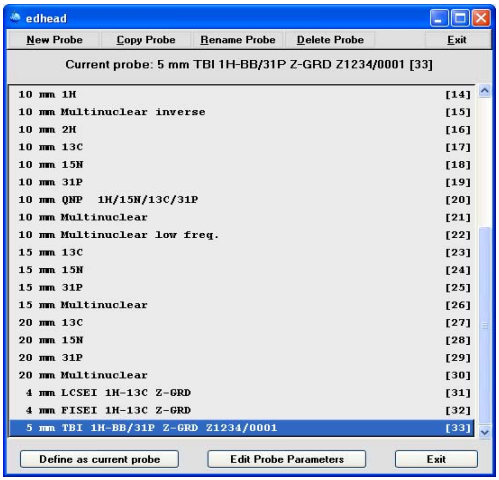
While expinstall will be executed you are able to continue with next configuration program.

- Continue with ***edsolv***



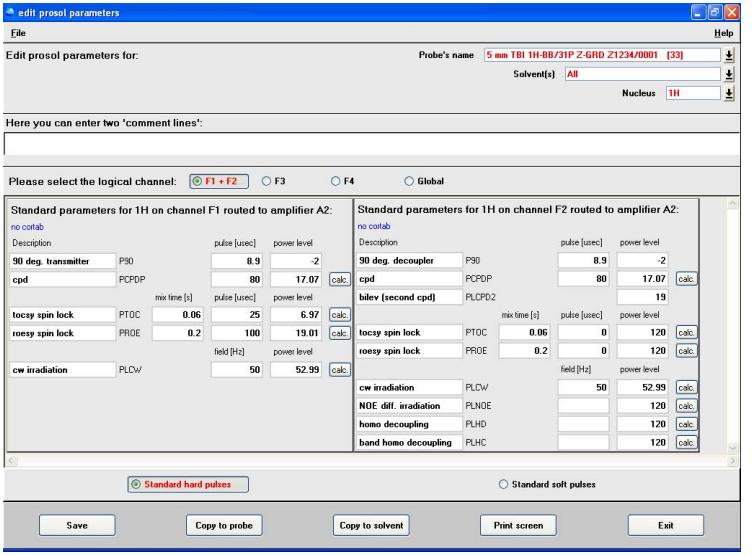
Check the list of lock solvents and click ***Save*** if it is correct → Click ***Close***

- Continue with ***edhead***



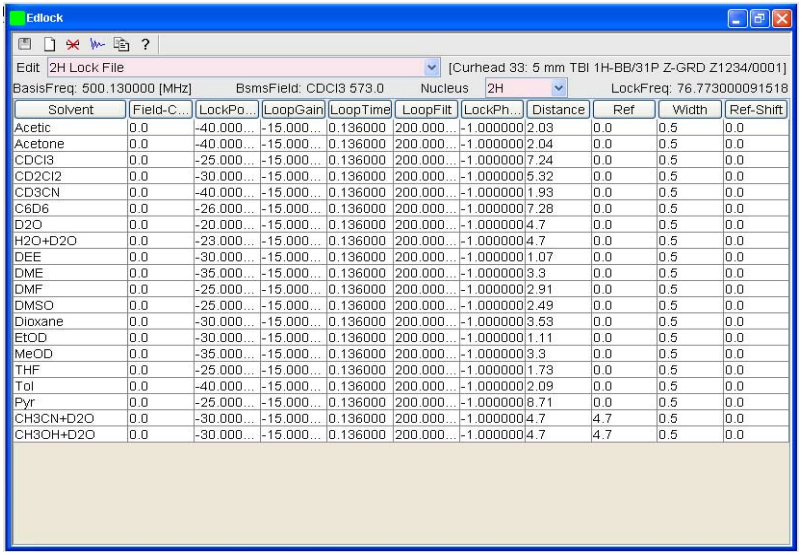
Select the current probe, click the button ***Define as current probe*** → Click ***Exit***

- Continue with ***edprosol***


edit prosol parameters
File
Help
Edit prosol parameters for:
Probe's name 5 mm TBI 1H-BB/31P Z-GRD Z1234/0001 [33]
Solvent(s) All
Nucleus 1H
Here you can enter two 'comment lines':
Please select the logical channel: F1 + F2 F3 F4 Global
Standard parameters for 1H on channel F1 routed to amplifier A2:
Standard parameters for 1H on channel F2 routed to amplifier A2:
Standard hard pulses
Standard soft pulses
Save
Copy to probe
Copy to solvent
Print screen
Exit

Check the parameters for your favorite nuclei, change them and calculate them, if necessary → Click ***Save*** to store to disk → Click ***Exit***

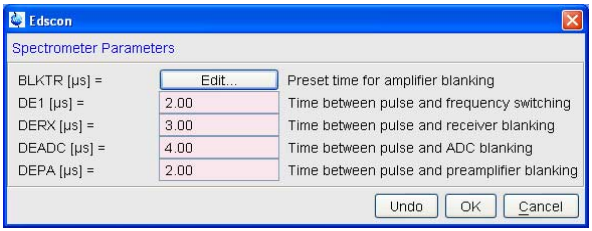
- Continue with ***edlock***



Solvent	Field-C...	LockPo...	LoopGain	LoopTime	LoopFilt	LockPh...	Distance	Ref	Width	Ref-Shift
Acetic	0.0	-40.000...	-15.000...	0.136000	200.000...	-1.000000	2.03	0.0	0.5	0.0
Acetone	0.0	-40.000...	-15.000...	0.136000	200.000...	-1.000000	2.04	0.0	0.5	0.0
CDCl3	0.0	-25.000...	-15.000...	0.136000	200.000...	-1.000000	7.24	0.0	0.5	0.0
CD2Cl2	0.0	-30.000...	-15.000...	0.136000	200.000...	-1.000000	5.32	0.0	0.5	0.0
CD3CN	0.0	-40.000...	-15.000...	0.136000	200.000...	-1.000000	1.93	0.0	0.5	0.0
C6D6	0.0	-26.000...	-15.000...	0.136000	200.000...	-1.000000	7.28	0.0	0.5	0.0
D2O	0.0	-20.000...	-15.000...	0.136000	200.000...	-1.000000	4.7	0.0	0.5	0.0
H2O+D2O	0.0	-23.000...	-15.000...	0.136000	200.000...	-1.000000	4.7	0.0	0.5	0.0
DEE	0.0	-30.000...	-15.000...	0.136000	200.000...	-1.000000	1.07	0.0	0.5	0.0
DME	0.0	-35.000...	-15.000...	0.136000	200.000...	-1.000000	3.3	0.0	0.5	0.0
DMF	0.0	-25.000...	-15.000...	0.136000	200.000...	-1.000000	2.91	0.0	0.5	0.0
DMSO	0.0	-25.000...	-15.000...	0.136000	200.000...	-1.000000	2.49	0.0	0.5	0.0
Dioxane	0.0	-30.000...	-15.000...	0.136000	200.000...	-1.000000	3.53	0.0	0.5	0.0
EtOD	0.0	-30.000...	-15.000...	0.136000	200.000...	-1.000000	1.11	0.0	0.5	0.0
MeOD	0.0	-35.000...	-15.000...	0.136000	200.000...	-1.000000	3.3	0.0	0.5	0.0
THF	0.0	-25.000...	-15.000...	0.136000	200.000...	-1.000000	1.73	0.0	0.5	0.0
Tol	0.0	-40.000...	-15.000...	0.136000	200.000...	-1.000000	2.09	0.0	0.5	0.0
Pyr	0.0	-25.000...	-15.000...	0.136000	200.000...	-1.000000	8.71	0.0	0.5	0.0
CH3CN+D2O	0.0	-30.000...	-15.000...	0.136000	200.000...	-1.000000	4.7	4.7	0.5	0.0
CH3OH+D2O	0.0	-30.000...	-15.000...	0.136000	200.000...	-1.000000	4.7	4.7	0.5	0.0

Check the lock table values (field, lock phase, ...), change them. Click ***Save***. To close the window, click on the ***X*** in the right corner.

- Continue with ***edscon***


Edscon
Spectrometer Parameters
BLKTR [µs] = Edit... Preset time for amplifier blanking
DE1 [µs] = 2.00 Time between pulse and frequency switching
DERX [µs] = 3.00 Time between pulse and receiver blanking
DEADC [µs] = 4.00 Time between pulse and ADC blanking
DEPA [µs] = 2.00 Time between pulse and preamplifier blanking
Undo
OK
Cancel

Check the spectrometer constants, change it and click ***Save*** if necessary, otherwise click ***Cancel***

After ***cf, expinstall***,... have finished insert a sample and make sure that you can lock on the lock solvent. Type ***ii*** and read with ***rpar*** a standard proton parameter file, type ***getprosol*** and ***rga*** and collect a normal ^{1}H NMR spectrum.

8.1.2 If you want to configure a processing-PC like your spectrometer-PC:

If the PC does not control a spectrometer but is used in connection with a particular spectrometer, e.g. for setting up experiments, processing and or plotting, you should configure it as that spectrometer (see FAQ 210 on www.bruker-biospin.de): for example the spectrometer is a AV300 configured with the name 'av300'. Do the following.

a) Copy the configuration directory '<TOPSPINHOME>/conf/instr/av300' from the spectrometer AV300 to the workstation.

b) On the workstation paste this 'av300' directory to '<TOPSPINHOME>/conf/instr'.

(most likely this is the path: c:\Bruker\TopSpin\conf\instr)

You can use the nmr_save AU program to transfer the configuration (see chapter 8.7).

a) Start TOPSPIN as Administrator.

b) Open a dataset

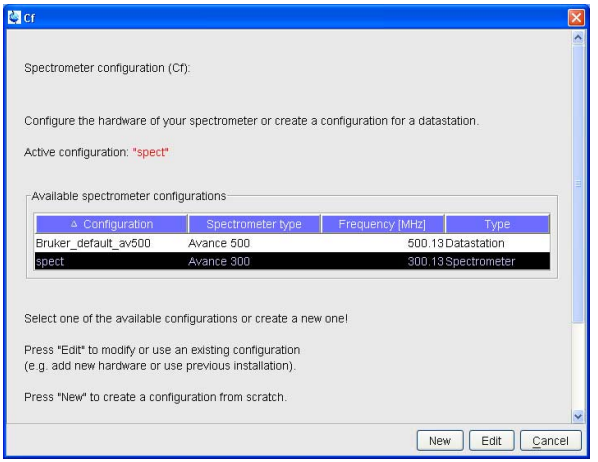
- Type ***new*** and create a new dataset.
- You can also select a dataset (e.g. *exam1d_1h*) acquired with another TOPSPIN or XWIN-NMR version.

c) Enter ***cf*** (The command ***cf*** now configures the software according to the hardware of your spectrometer):

a) A window will appear:
Password request. Please enter the NMR administration password

Type in the NMR ADMINISTRATION PASSWORD. Click **OK**.

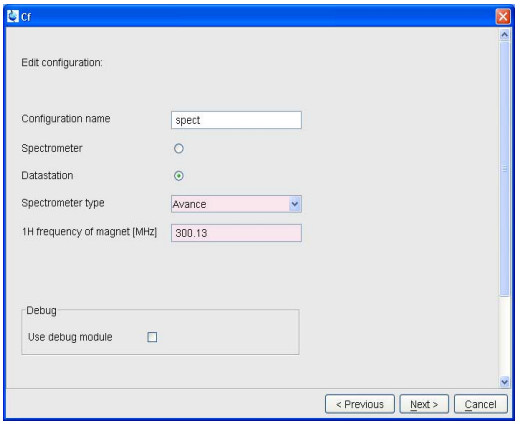
b) A window will appear:.



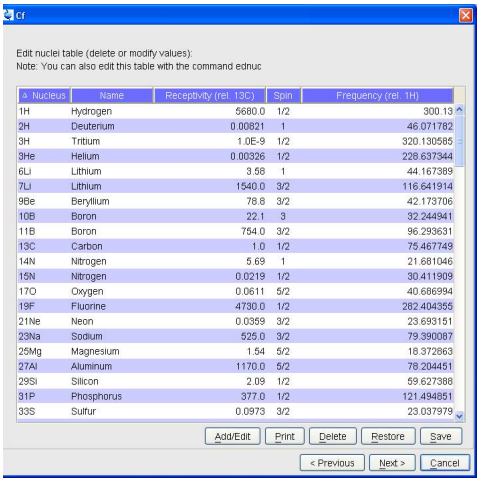
Press "Edit" to confirm this configuration.

c) A window will appear:

The selected configuration is displayed. Choose Datastation to configure your PC as a datastation.

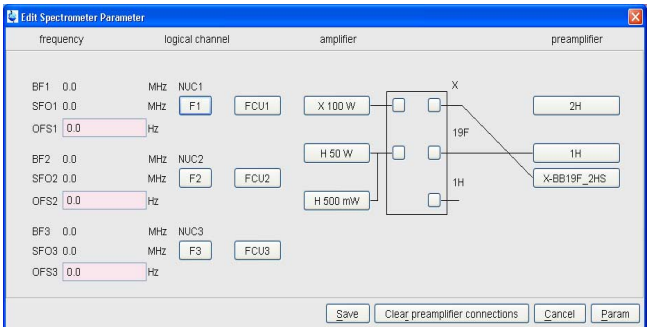


d) The *nuclei-table* appear.

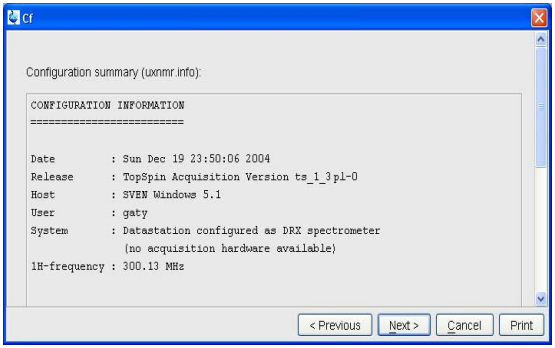

Cr
Edit nuclei table (delete or modify values):
Note: You can also edit this table with the command ednuc
Nucleus | Name | Receptivity (rel. 13C) | Spin | Frequency (rel. 1H)
1H Hydrogen 5680.0 1/2 300.13
2H Deuterium 0.00821 1 46.071782
3H Tritium 1.0E-9 1/2 320.130585
3He Helium 0.00326 1/2 228.637344
6Li Lithium 3.58 1 44.167389
7Li Lithium 1540.0 3/2 116.641914
9Be Beryllium 78.8 3/2 42.173706
10B Boron 22.1 3 32.244941
11B Boron 754.0 3/2 96.293631
13C Carbon 1.0 1/2 75.467749
14N Nitrogen 5.69 1 21.681046
15N Nitrogen 0.0219 1/2 30.411909
17O Oxygen 0.0611 5/2 40.686994
19F Fluorine 4730.0 1/2 282.404355
21Ne Neon 0.0359 3/2 23.693151
23Na Sodium 525.0 3/2 79.390087
25Mg Magnesium 1.54 5/2 18.372863
27Al Aluminum 1170.0 5/2 78.204451
29Si Silicon 2.09 1/2 59.627388
31P Phosphorus 377.0 1/2 121.494851
33S Sulfur 0.0973 3/2 23.037979
Add/Edit
Print
Delete
Restore
Save
< Previous
Next >
Cancel

Check if the frequency of the nuclei are set correctly and click ***Save*** (If in doubt click ***Restore*** then click ***Save***)

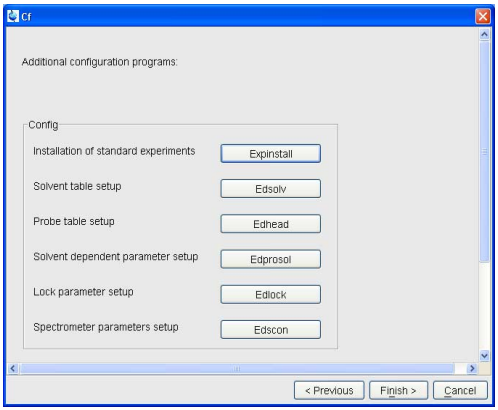
e) A window 'Edit spectrometer configuration will appear: click ***Save***..



f) The results of ***cf*** appears in a text window → click ***Next.***.



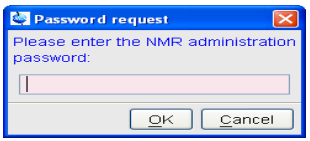
After finishing cf window '*Additional configuration programs*' will appear showing a list of configuration steps. .



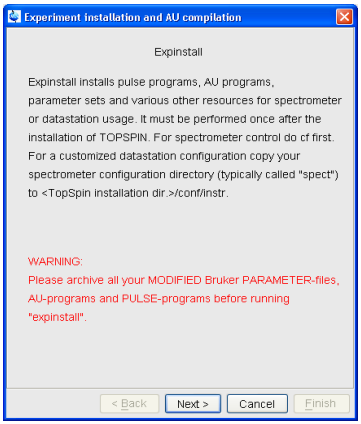
Accept the default selection and click on the buttons (You will be asked for the NMR ADMINISTRATION PASSWORD a couple of times):

- Continue with ***expinstall***

a) Type in the NMR ADMINISTRATION PASSWORD and **OK**

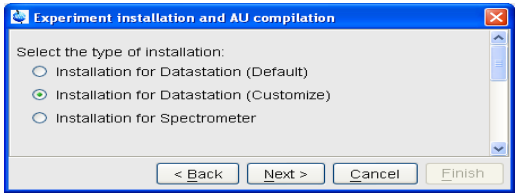


b) Click **Next** if you either have no modified Bruker BioSpin-Parameterfiles


Experiment installation and AU compilation
Expinstall
Expinstall installs pulse programs, AU programs, parameter sets and various other resources for spectrometer or datastation usage. It must be performed once after the installation of TOPSPIN. For spectrometer control do cf first. For a customized datastation configuration copy your spectrometer configuration directory (typically called "spect") to <TopSpin installation dir.>/conf/instr.
WARNING:
Please archive all your MODIFIED Bruker PARAMETER-files, AU-programs and PULSE-programs before running "expinstall".
< Back
Next >
Cancel
Finish

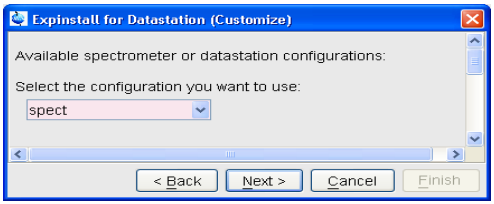
AU-programs and Pulse-programs or if you have archive them in a different directory. Your individual Parameterfiles, AU-programs and Pulse-programs that have different names to the original Bruker BioSpin files will not be destroyed during the installation

c) In the appearing window → Check *Installation for Datastation (Customize)* → Click ***Next***

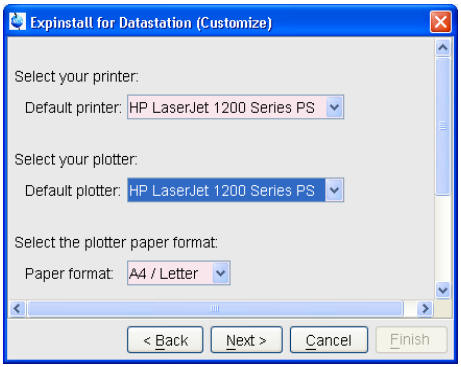


d) In the appearing window → Check *High Resolution Systems* → Click ***Next***

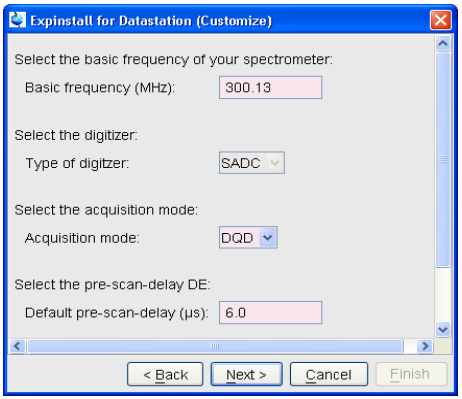
e) In the appearing dialog box → Select the spectrometer configuration name → Click ***Next***



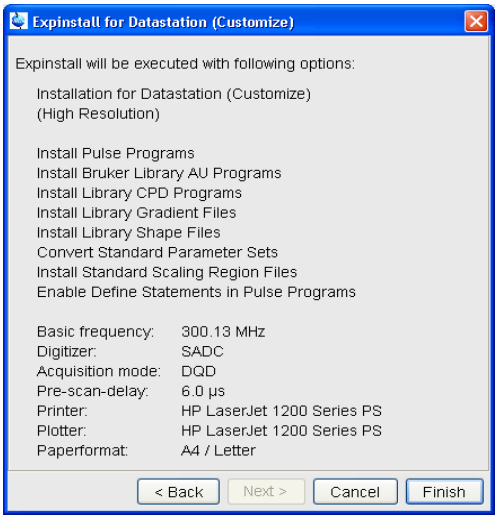
f) In the appearing dialog box → Select the default printer and plotter and the desired paper format → Click ***Next***


Expinstall for Datastation (Customize)
Select your printer:
Default printer: HP LaserJet 1200 Series PS
Select your plotter:
Default plotter: HP LaserJet 1200 Series PS
Select the plotter paper format:
Paper format: A4 / Letter
< Back
Next >
Cancel
Finish

g) In the appearing window → Click ***Next***



h) In the appearing information box → Check the configuration selection and, if it is correct → Click ***Finish***



The installation of the selected items, will start now. Wait until this process has finished.

For more details on ***expinstall***, please refer to the description of this command in the Acquisition Reference manual.

8.1.3 If you want to use a default configuration on a datastation

A default configuration can be used on a datastation. It is automatically performed (no ***cf*** required) during the installation of TOPSPIN on a new computer, a new disk or in a new TOPSPIN installation directory. The default configuration name is *Bruker_default_av500* and corresponds to a Avance 500 MHz spectrometer.

For manual or interactive data processing, the automatic default configuration is sufficient. If, however, you want to use AU programs, you must execute ***expinstall*** once, selecting *Installation for Datastation (Default).*

8.1.4 If you do not know the configuration of your spectrometer

If you do not have any spectrometer configuration information, e. g. after a headcrash, then you have to recreate the configuration information.

In this situation there are two possibilities:

a) your spectrometer has a standard configuration

b) your spectrometer has a non-standard configuration

Case a)

If your spectrometer has a standard configuration, then you can easily do ***cf*** and if you give the correct information for the '*Type of Spectrometer*' you will get the correct list of your hardware in the '*RS232 table*'. You only have to type in the correct tty's of the interfaces.

Case b)

If your D*X spectrometer has a non-standard configuration, then the hardware configuration is read during the ***cf*** from the file 'hardware_list' file in the directory

<TOPSPINHOME>\conf\instr\<spectrometer-name>

TOPSPIN 1.3 offers the default file 'hardware.exam' which contains a list of all available hardware components which are important for the ***cf*** command. This file was generated in XWIN-NMR with the command ***cf makelist***, now it is available in:

<TOPSPINHOME>\conf\instr

- Open this file with a text editor, e. g. Notepad, and delete all lines except those that describe the hardware components of your spectrometer. You can get this information in the following way:
  Check the list in the file 'hardware.exam' with the components of your spectrometer and/or with the Bruker BioSpin delivery note(s). Please carefully check the PN-C/D/E and ECL numbers of the components

- **Save** and **exit** from 'hardware.exam'
- Copy the modified file hardware.exam' into the directory
  <TOPSPINHOME>\conf\instr\<spect>
- Rename the file
  <TOPSPINHOME>\conf\instr\<spect>/hardware.exam to
  <TOPSPINHOME>\conf\instr\<spect>/hardware_list

8.1.5 If you added a new hardware component to your spectrometer

If you want to add a new hardware component it is recommended to order somebody of your local Bruker BioSpin office to do this for you.

If you have to add a new hardware component to the configuration file of the software, do the following:

TOPSPIN 1.3 offers the default file '`hardware.exam`' which contains a list of all available hardware components which are important for the ***`cf`*** command. This file was generated in XWIN-NMR with the command ***`cf makelist`***, now it is available in:

`<TOPSPINHOME>\conf\instr`

- Open this file with a text editor, e. g. kedit, and search and copy these line(s) that describe the new hardware component(s). Please carefully check the PN-C/D/E and ECL number(s) of the component(s).

- Copy the file
  `<TOPSPINHOME>/conf/instr/spect/hardware_list` to
  `<TOPSPINHOME>/conf/instr/spect/hardware_list_sav`
- Open the file
  `<TOPSPINHOME>/conf/instr/spect/hardware_list`
  and paste the new entries to the correct positions.

8.2 Take over the configuration of XWIN-NMR or TOPSPIN into TOPSPIN 1.3

The decision how to install TOPSPIN is very important in case you have already XWIN-NMR or TOPSPIN installed on the same or another PC. If so, you might will take over the configuration of XWIN-NMR or TOPSPIN 1.2 into TOPSPIN 1.3 because of:

- in case the XWIN-NMR/TOPSPIN installation was used for controlling a spectrometer there are very important configuration files like the spectrometer configuration, shim files, your own pulse programs, parameter sets, etc.
- if XWIN-NMR/TOPSPIN was used for processing only there can be also very important configuration files like AU programs, macros, plot layouts etc.

! *Note: Transferring files could cause permission problems especially if they are transferred from one PC to another.*

8.2.1 Take over the configuration on the same PC

If TOPSPIN 1.3 is installed parallel to TOPSPIN 1.2 or XWIN-NMR, the AU program ***nmr_save*** can be used to take over the configuration of XWIN-NMR/TOPSPIN.

You can take over the configuration during the Installation of TOPSPIN 1.3 (see chapter 6.4) or after the installation with the AU program ***nmr_save***.

If you like to get more information about the command ***nmr_save*** refer to chapter 8.7.

Insert the TOPSPIN DVD and start installation. You will be asked to define the installation path. Accept the default or choose another one but not the XWIN-NMR installation directory. During the installation you will be asked if you want to import a spectrometer configuration. If you want to take over the configuration after installation is finished, start TOPSPIN

- and type in the command:

  nmr_save

- or click

  Options → Spectrometer Tools → Save/Restore configuration

A window 'Password request' will appear. Please enter the NMR administration password and click ***OK***.

A window 'NMR_Save' appears. Please check the 'Location of Backup file' (default: `<TOPSPINHOME>\nmr_backup`). Enter the location of the installation to be saved (e.g. `C:\Bruker\XWIN-NMR`). Click on ***Save***.

This will create a tar file of all necessary information from the XWIN-NMR installation. The tar-file is called `nmr_backup.tar` and will be stored in the directory:

`<TOPSPINHOME>\nmr_backup`

To take over this information into TOPSPIN, please enter the restore destination (e.g. `<TOPSPINHOME>`) and click on ***Restore***.

After this process is finished, execute ***cf***.

8.2.2 Take over the configuration on another PC

Before you start installation of TOPSPIN on PC-A you have to copy the two directories:

`<XWINNMRHOME>/conf` and `<XWINNMRHOME>/exp`

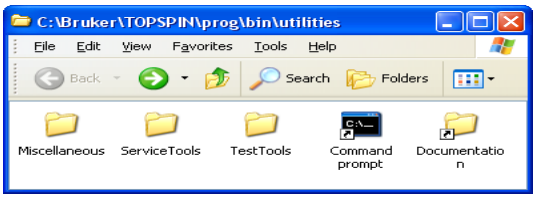
from the XWIN-NMR installation on the PC-B into the directory where TOPSPIN will be installed. The default installation directory of TOPSPIN is for Windows:

`C:\Bruker\Topspin`

In case you will use the default installation path you have to create these directories and as a second step copy the two directories `conf` and `exp` into them. After these two directories are available on PC-A you can start the TOPSPIN installation.

8.3 How to use the Bruker Utilities Folder

After a successful installation of the TOPSPIN, you will find a new folder on every user's desktop named 'Bruker Utilities'. Double click on the folder to see its contents:

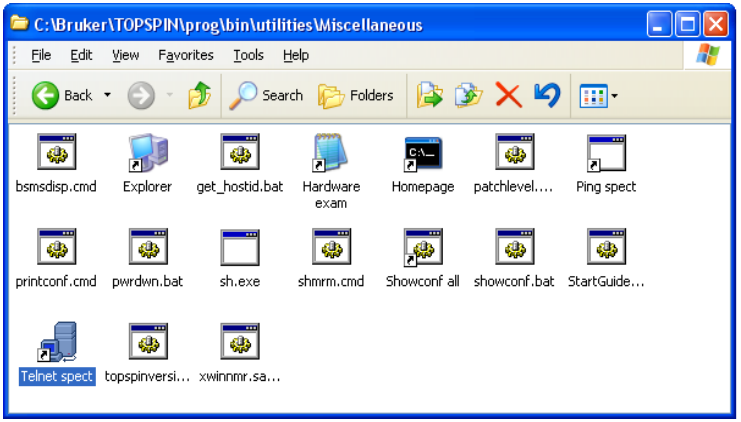


or

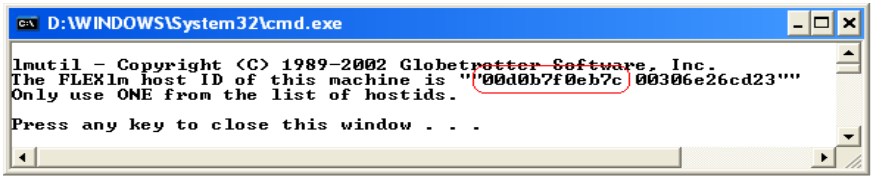
1. Click **Start** → **All Programs** → **Bruker TOPSPIN** → **Bruker TOPSPIN x.y** → **Bruker Utilities**
2. A window '*Bruker Utilities*' appears.

In this Utilities folder, you will find commands and applications that you might need when running and configuring a spectrometer. You can see the command prompt right there: just double click on it to get to the prompt.

The other tools are stored in three categories as shown above. You can double click on each of the folders to have them opened up to show their treasures:



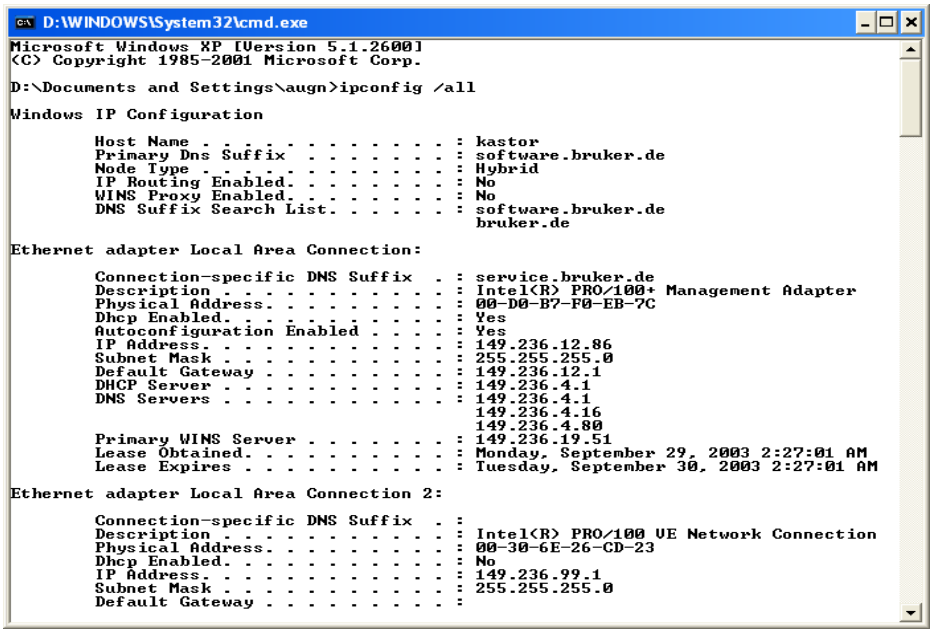
Each of them (our example here is 'miscellaneous') have a number of batches or executables, or plain commands that you can run by just double clicking on the respective icon. For example, to see the system ID of the current PC you can just double-click on the icon called 'get_hostid'. It will open a text window and deliver the system ID you need to know when you apply for TOPSPIN license (encircled):


D:\WINDOWS\System32\cmd.exe
lmutil - Copyright (C) 1989-2002 Globetrotter Software, Inc.
The FLEXlm host ID of this machine is ""00d0b7f0eb7c 00306e26cd23""
Only use ONE from the list of hostids.
Press any key to close this window . . .

If you press any key, the window will be closed again.

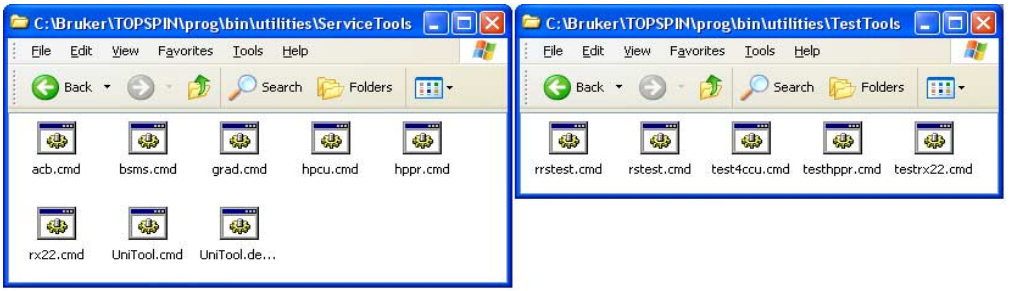
As you can see from the next screen (produced by the command `ipconfig /all` in a command prompt) flexlm takes the address of one of the Ethernet cards in the PC. Which one is used depends on the binding order of the two cards. You

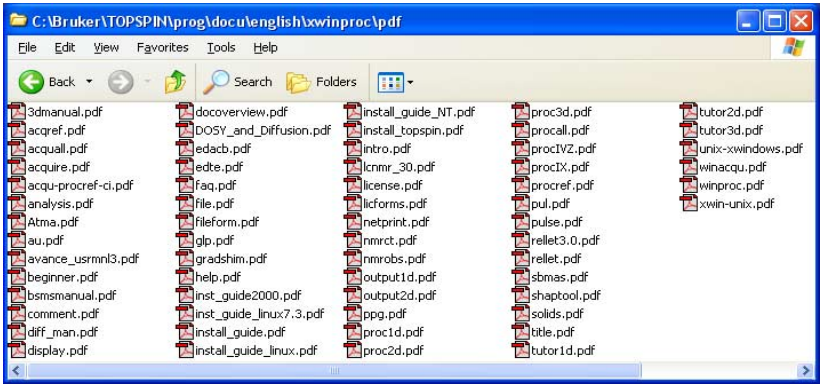
can check the binding by clicking the icon from the Control Panel.


D:\WINDOWS\System32\cmd.exe
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.
D:\Documents and Settings\augn>ipconfig /all
Windows IP Configuration
Host Name . . . . . : kastor
Primary Dns Suffix . . . . . : software.bruker.de
Node Type . . . . . : Hybrid
IP Routing Enabled. . . . . : No
WINS Proxy Enabled. . . . . : No
DNS Suffix Search List. . . . . : software.bruker.de
bruker.de
Ethernet adapter Local Area Connection:
Connection-specific DNS Suffix . : service.bruker.de
Description . . . . . : Intel(R) PRO/100+ Management Adapter
Physical Address. . . . . : 00-D0-B7-F0-EB-7C
Dhcp Enabled. . . . . : Yes
Autoconfiguration Enabled . . . . : Yes
IP Address. . . . . : 149.236.12.86
Subnet Mask . . . . . : 255.255.255.0
Default Gateway . . . . . : 149.236.12.1
DHCP Server . . . . . : 149.236.4.1
DNS Servers . . . . . : 149.236.4.1
149.236.4.16
149.236.4.80
Primary WINS Server . . . . . : 149.236.19.51
Lease Obtained. . . . . : Monday, September 29, 2003 2:27:01 AM
Lease Expires . . . . . : Tuesday, September 30, 2003 2:27:01 AM
Ethernet adapter Local Area Connection 2:
Connection-specific DNS Suffix . :
Description . . . . . : Intel(R) PRO/100 VE Network Connection
Physical Address. . . . . : 00-30-6E-26-CD-23
Dhcp Enabled. . . . . : No
IP Address. . . . . : 149.236.99.1
Subnet Mask . . . . . : 255.255.255.0
Default Gateway . . . . . :

Another interesting tool in the 'miscellaneous' section actually issues commands to the CCU rather than to the PC. One of the items is 'pwrdwn' in this category that logs in to CCU and issues the UNIX command that powers down the CCU. All YOU do is double click on it and watch it do the rest.

The other categories are 'Test Tools', Service Tools and Documentation. You can just double-click the appropriate icon and the command-shell and tool programs will start up automatically.:





8.4 Configuring the BSMS-Keyboard

For a full description how to configure the BSMS-Keyboard see your

- hard copy of '*BSMS-User Manual*' or
- the respective entry on the '*BASH' CD-ROM*' (Order Number Z36541)

A configuring step that should be done periodically is the spin rate calibration. For this you have to go into the ***Menu*** mode of your BSMS keyboard. Press simultaneously ***2nd*** and ***Y^3***, then rotate the control knob as long as you see ***1.Sample*** in the display, press ***2nd*** to go into this directory. The display will show ***1.1 Spin calib.*** press ***2nd*** to start this process and wait for ~ 3 minutes.

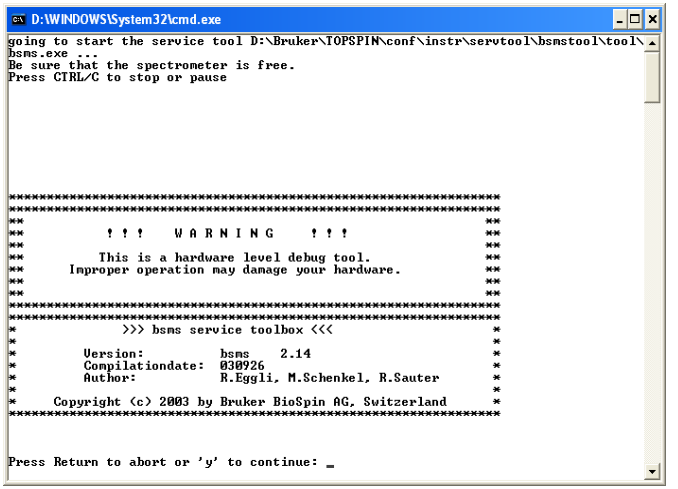
In this Menu mode, you can also define the helium warning level. If the liquid helium reaches the critical point, the BSMS-Keyboard starts beeping. A special password, the so called security code, is required to be able to change the setting.For an additional possibility to get a warning about a low helium level see chapter 21.2. If in doubt about the setting, contact your service representative.

8.5 Firmware update of the spectrometer hardware

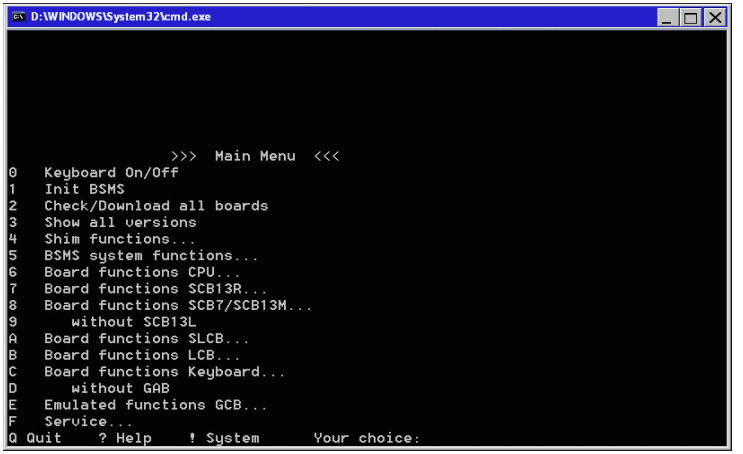
This chapter describes how to update the firmware of spectrometer components. This is only necessary if the cf command has crashed and popped up a message window which informs that you have to do a firmware update of a certain component.

It is strongly recommended to do the firmware update only in this case, because the hardware component could become unusable if the update was done incorrectly.

1. Start the '***Service Tools***' of the '***Bruker Utilities***' to check the firmware version of your spectrometer hardware.
2. Double click on an icon starts an automatic procedure that opens a command prompt. The following example shows the check of the '*bsms-service tool*'


D:\WINDOWS\System32\cmd.exe
going to start the service tool D:\Bruker\TOPSPIN\conf\instr\servtool\bsmstool\tool\bsms.exe ...
Be sure that the spectrometer is free.
Press CTRL/C to stop or pause
! ! ! WARNING ! ! !
This is a hardware level debug tool.
Improper operation may damage your hardware.
>>> bsms service toolbox <<<
Version: bsms 2.14
Compilationdate: 030926
Author: R.Eggli, M.Schenkel, R.Sauter
Copyright (c) 2003 by Bruker BioSpin AG, Switzerland
Press Return to abort or 'y' to continue:

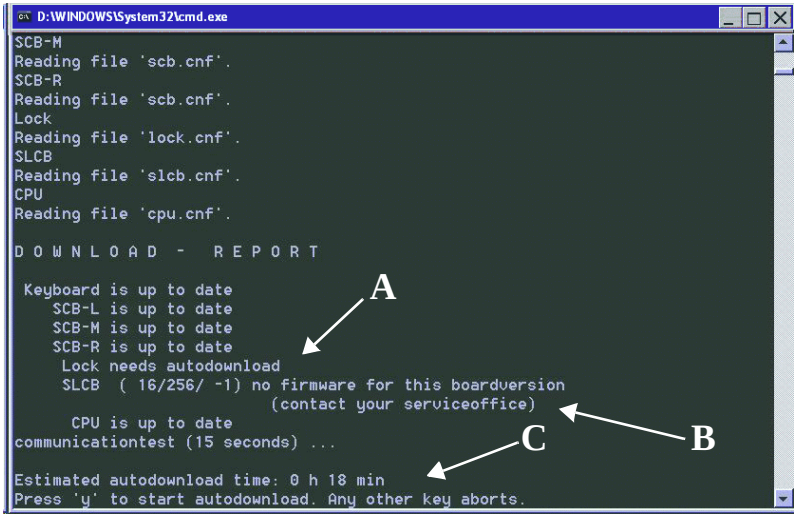
3. Type ***y*** → **ENTER**
4. A dialog comes up in the command prompt



5. To check and eventually download a new firmware (from TOPSPIN)

- type ***2***→ **ENTER**

  The check starts and ends for example as shown in the following picture

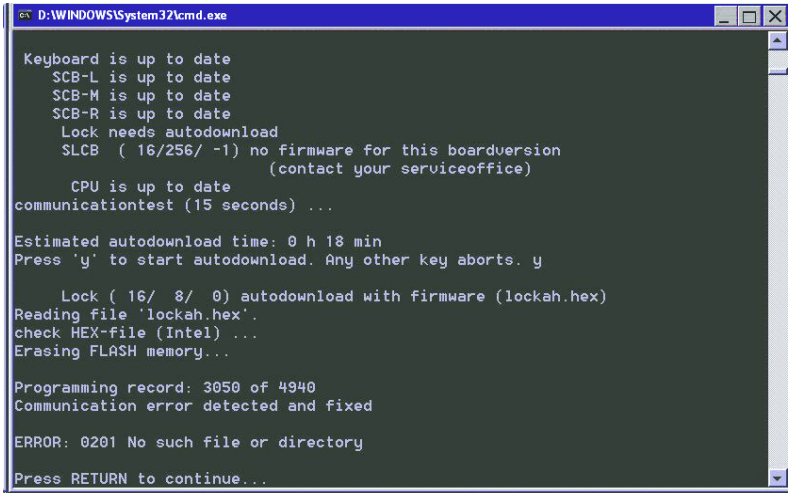


  - if there is a problem with a component you get an information to contact your serviceoffice (B)
  - if you need a firmware update you will get a message (A) with the length of time for the download (C). It is recommended to do the download as soon as possible.

6. Press ***y*** → **ENTER** to start the download

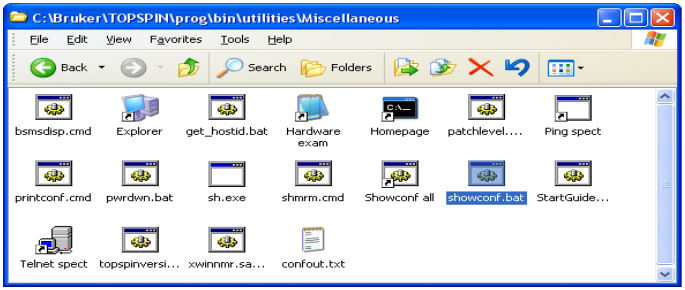
During the download it is absolutely necessary that spectrometer and PC are not disturbed! Make sure that no one pulls a cable out of the spectrometer or uses Windows XP parallel! (Yes, we know this seems very improbable, but if the download would crash your board might be unusable afterwards)

- A normal error during downloading the new firmware (see above) requires to do the download once again!
- If you have done a download of newer firmware, you have to do ***cf*** again!
- If you do not need any downloads you can follow the instructions in the command prompt to end this tool.

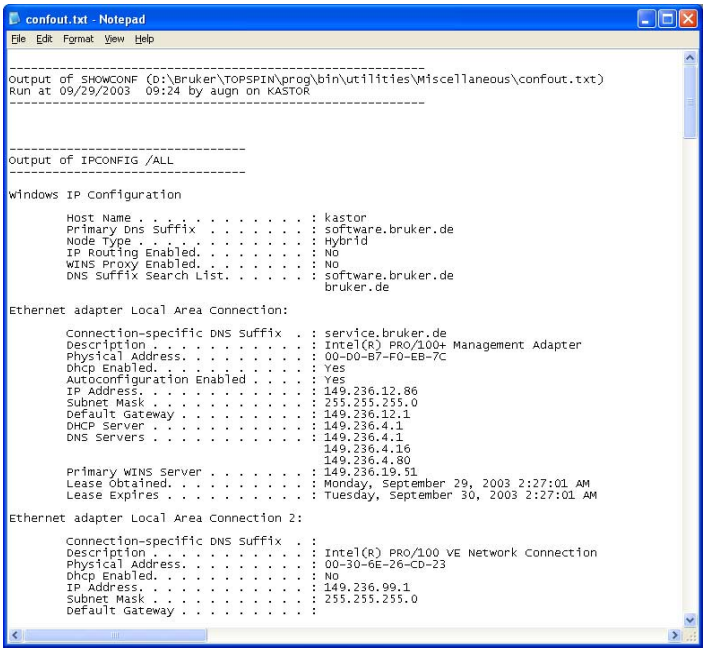

D:\WINDOWS\System32\cmd.exe
Keyboard is up to date
SCB-L is up to date
SCB-M is up to date
SCB-R is up to date
Lock needs autodownload
SLCB (16/256/ -1) no firmware for this boardversion
(contact your serviceoffice)
CPU is up to date
communicationtest (15 seconds) ...
Estimated autodownload time: 0 h 18 min
Press 'y' to start autodownload. Any other key aborts. y
Lock (16/ 8/ 0) autodownload with firmware (lockah.hex)
Reading file 'lockah.hex'.
check HEX-file (Intel) ...
Erasing FLASH memory...
Programming record: 3050 of 4940
Communication error detected and fixed
ERROR: 0201 No such file or directory
Press RETURN to continue...

8.6 A log of the entire system configuration

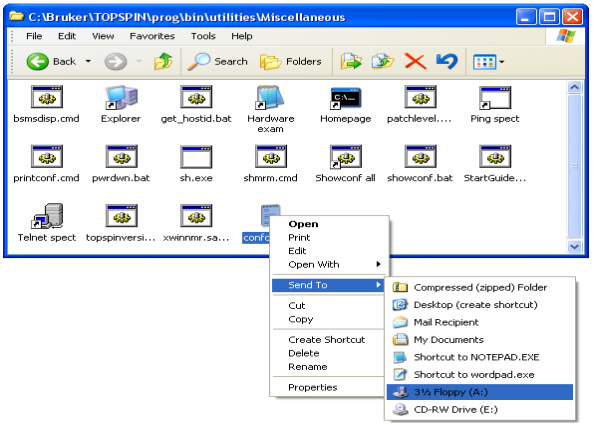
The ***showconf*** command provides you with various information about your hardware and software, both of the PC and of the spectrometer. Here is how showconf works: Go to the folder ***Bruker Utilities*** → ***Miscellaneous*** → double-click on the ***showconf*** icon and wait about 2 minutes until it has finished. After that showconf has produced a file called `confout.txt` that contains all you need. `Confout.txt` is located next to the showconf batch after the first execution and you edit it from there:



Just double click on the confout icon to call the appropriate editor:


confout.txt - Notepad
File Edit Format View Help
Output of SHOWCONF (D:\Bruker\TOPSPIN\prog\bin\utilities\Miscellaneous\confout.txt)
Run at 09/29/2003 09:24 by augn on KASTOR
Output of IPCONFIG /ALL
Windows IP Configuration
Host Name . . . . . : kastor
Primary Dns Suffix . . . . . : software.bruker.de
Node Type . . . . . : Hybrid
IP Routing Enabled. . . . . : No
WINS Proxy Enabled. . . . . : No
DNS Suffix Search List. . . . . : software.bruker.de
bruker.de
Ethernet adapter Local Area Connection:
Connection-specific DNS Suffix . : service.bruker.de
Description . . . . . : Intel(R) PRO/100+ Management Adapter
Physical Address. . . . . : 00-D0-B7-F0-EB-7C
Dhcp Enabled. . . . . : Yes
Autoconfiguration Enabled . . . . : Yes
IP Address. . . . . : 149.236.12.86
Subnet Mask . . . . . : 255.255.255.0
Default Gateway . . . . . : 149.236.12.1
DHCP Server . . . . . : 149.236.4.1
DNS Servers . . . . . : 149.236.4.1
149.236.4.16
149.236.4.80
Primary WINS Server . . . . . : 149.236.19.51
Lease Obtained. . . . . : Monday, September 29, 2003 2:27:01 AM
Lease Expires . . . . . : Tuesday, September 30, 2003 2:27:01 AM
Ethernet adapter Local Area Connection 2:
Connection-specific DNS Suffix . :
Description . . . . . : Intel(R) PRO/100 VE Network Connection
Physical Address. . . . . : 00-30-6E-26-CD-23
Dhcp Enabled. . . . . : No
IP Address. . . . . : 149.236.99.1
Subnet Mask . . . . . : 255.255.255.0
Default Gateway . . . . . :

The easiest way to copy it on a diskette is right from within the miscellaneous-folder: Right-click on the `confout`-icon and select 'send to' and then A:



The size of this report is mostly less then 100 kbytes.

DO KEEP A COPY OF THIS FILE IN A SAFE PLACE!

8.7 Backup of VIFs (=Very Important Files) with nmr_save

It is not only necessary to create some backups for the operating system like Boot Disks and to store the acquired datasets.

! it is strictly recommended to create a frequently backup of the 'VIFs' - the 'Very Important Files' of the configuration of TOPSPIN.

There are many reasons like e. g. head crash or theft of the hard disk that makes it important that a weekly or monthly backup is made of important data, so that you would be able to restore the spectrometer configuration in a very short time.

TOPSPIN offers an AU program[1] (***nmr_save***) for saving those important files that are not delivered by BRUKER. This AU program can save and extract user specific data from the TOPSPINHOME directory and puts them into a tar-file. Files that start with an "." are ignored.

The AU program can be started as follows:

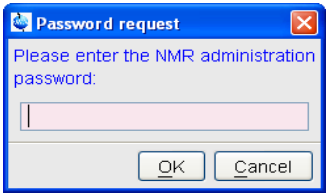
- Start TOPSPIN and type in the command:

  nmr_save

- or start TOPSPIN and click

  Options → Spectrometer Tools → Save/Restore configuration

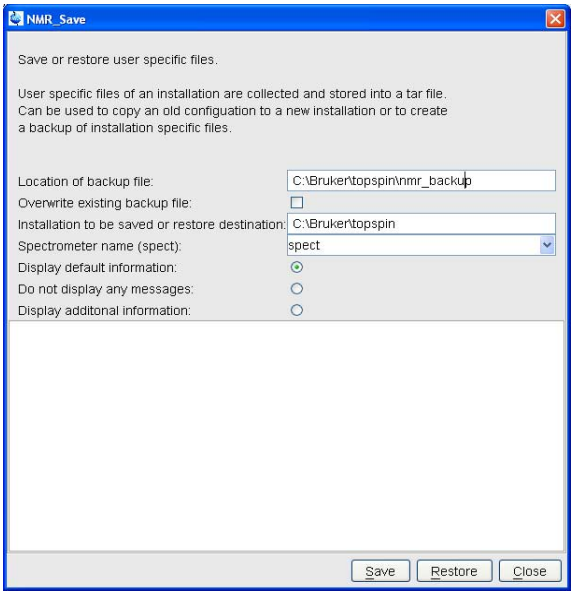
A window 'Password request' will appear.



Please enter the NMR administration password and click ***OK***.

1. BRUKER also offers a script (xwinnmr.save) which can be used for saving the 'VIF's (see chapter 21.4).

A window 'NMR_Save' will appear.


NMR_Save
Save or restore user specific files.
User specific files of an installation are collected and stored into a tar file.
Can be used to copy an old configuation to a new installation or to create
a backup of installation specific files.
Location of backup file:
C:\Bruker\topspin\nmr_backup
Overwrite existing backup file:
Installation to be saved or restore destination:
C:\Bruker\topspin
Spectrometer name (spect):
spect
Display default information:
Do not display any messages:
Display additonal information:
Save
Restore
Close

Please check the 'Location of Backup file' (the default is: `<TOPSPIN-HOME>\nmr_backup`). Enter the location of the installation to be saved (the default is: `<TOPSPINHOME>`) and click on ***Save***.

This will create a tar file of all necessary information from respective installation. The tar-file is called `nmr_backup.tar` and will be stored in the directory:

`<TOPSPINHOME>\nmr_backup`

Files and directories will be saved into the special tar-file `nmr_backup.tar` which is, by default, in the directory `TOPSPINHOME/nmr_backup`.

The following directories are saved completely (hidden files are ignored!):

`<TOPSPINHOME>/exp/stan/nmr/lists/group/`

`<TOPSPINHOME>/exp/stan/nmr/lists/scm/`

`<TOPSPINHOME>/exp/stan/nmr/lists/bsms/`

`<TOPSPINHOME>/exp/stan/nmr/lists/mac/`

`<TOPSPINHOME>/exp/stan/nmr/lists/f1/`

`<TOPSPINHOME>/exp/stan/nmr/lists/ds/`

<TOPSPINHOME>/exp/stan/nmr/py/

<TOPSPINHOME>/prog/server/

<TOPSPINHOME>/conf/instr/probehead/

<TOPSPINHOME>/conf/instr/<spect>/prosol/

<TOPSPINHOME>/conf/instr/<spect>/cortab/

<TOPSPINHOME>/conf/instr/<spect>/inmrusers/

<TOPSPINHOME>/conf/instr/autoshim/refmaps/

<TOPSPINHOME>/data/final/nmr/protocolfiles/

<TOPSPINHOME>/QTP/

<spect> represents the current spectrometer name or the name specified explicitly when ***nmr_save*** is started.

From the following directories every file is saved that does not belong to the genuine Bruker distribution:

<TOPSPINHOME>/exp/stan/nmr/lists/pp/

<TOPSPINHOME>/exp/stan/nmr/lists/cpd/

<TOPSPINHOME>/exp/stan/nmr/lists/gp/

<TOPSPINHOME>/exp/stan/nmr/lists/wave/

<TOPSPINHOME>/exp/stan/nmr/au/scl/

<TOPSPINHOME>/exp/stan/nmr/au/src/

<TOPSPINHOME>/exp/stan/nmr/par/

<TOPSPINHOME>/plot/layouts/

<TOPSPINHOME>/prog/tcl/xwish3_scripts/

Additionally, the following files are also saved:

<TOPSPINHOME>/conf/instr/<spect>/uxnmr.par

<TOPSPINHOME>/conf/instr/<spect>/uxnmr.info

<TOPSPINHOME>/conf/instr/<spect>/specpar

<TOPSPINHOME>/conf/instr/<spect>/2Hlock

<TOPSPINHOME>/conf/instr/<spect>/nuclei

<TOPSPINHOME>/conf/instr/<spect>/best-nmr/CurrPushSolvent

<TOPSPINHOME>/conf/instr/<spect>/best-nmr/hardware.par
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/hardware.src
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/racks.src
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/scanner.src
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/solvents.add
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/solvents.add
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/solvents.use
<TOPSPINHOME>/conf/instr/<spect>/rs232_device/best
<TOPSPINHOME>/conf/instr/<spect>/rs232_device/bestscan
<TOPSPINHOME>/conf/instr/probehead
<TOPSPINHOME>/exp/stan/nmr/lists/solvents
<TOPSPINHOME>/exp/stan/nmr/lists/probeheads
<TOPSPINHOME>/conf/instr/<spect>/hardware_list
<TOPSPINHOME>/prog/logfiles/heliumlog
<TOPSPINHOME>/prog/logfiles/heliumlog.err
<LM_License_File>[1]

For safety reasons the tar-file will not be replaced by executing ***nmr_save*** once again. So if you like to use this AU program several times, you have to move the nmr_backup.tar file from the directory <TOPSPINHOME>/nmr_backup on a backup medium (floppy, CD ...) and then start the script once again or you have to select the 'Overwriting existing backup file' option.

The options for ***nmr_save*** are:

- ***Location of backup file:***
  absolute path where backup tar-file nmr_backup.tar will be created ('save option') or can be found ('restore option')
- ***Overwriting existing backup file:***
  overwrite existing nmr_backup.tar file

1. This is the environment variable for the license file, in a default installation this is: C:\flexlm\Bruker\licenses\license.dat

- ***Installation to be saved or restore destination:***
  a) absolute path to TOPSPIN/XWIN-NMR installation that should be saved.
  b) absolute path where backup tar-file will be extracted.
- ***Overwriting existing backup file:***
  overwrite existing nmr_backup.tar file
- ***Spectrometer name (spect):***
  name of the spectrometer configuration
- ***Display default information***:
  display the directories and files which will be saved
- ***Do not display any messages***:
  do not display any messages
- ***Display additional information***:
  display all files which will be saved

To take over this information into TOPSPIN, please start ***nmr_save***.

Enter the restore destination (e.g.: `<TOPSPINHOME>`) and click on ***Restore***.

Examples for backing up the current Topspin installation:

1. Default backup directory used:
   - Location of backup file: `<topspinhome>\nmr_backup` (e.g.: `C:\Bruker\TOPSPIN\nmr_backup`)
   - Installation to be saved or restore destination: `<topspinhome>` (e.g.: `C:\Bruker\TOPSPIN`)
   - Spectrometer name (spect): <spect> (e.g.: `spect`)
   - Click ***Save***
2. Default backup directory used, but the spectrometer directory spect_org is saved which is not the default being defined in `<TOPSPINHOME>/conf/instr/curinst`
   - Location of backup file: `<topspinhome>\nmr_backup`
   - Installation to be saved or restore destination: `<topspinhome>`
   - Spectrometer name (spect): spect_org

- Click ***Save***

3. /tmp as backup directory:
   - Location of backup file: `C:\tmp`
   - Installation to be saved or restore destination: `<topspinhome>`
   - Spectrometer name (spect): <spect>
   - Click ***Save***

Example for backing up the current XWIN-NMR installation (If TOPSPIN is parallel installed to XWIN-NMR):

1. To create a tar file of all important files and directories from the XWIN-NMR installation in `C:\Bruker\XWIN-NMR` and `TopSpin` installation in `C:\Bruker\TOPSPIN`:
   - Location of backup file: `C:\Bruker\TOPSPIN\nmr_backup`
   - Installation to be saved or restore destination: `<topspinhome>` (e.g.: `C:\Bruker\XWIN-NMR`)
   - Spectrometer name (spect): <spect> (e.g.: `spect`)
   - Click ***Save***

Examples for restoring the backup file

1. Restoring the backup file `C:\Bruker\TOPSPIN\nmr_backup\nmr_backup.tar` into the Topspin home directory (default):
   - Location of backup file: `C:\Bruker\TOPSPIN\nmr_backup`
   - Installation to be saved or restore destination: `C:\Bruker\TOPSPIN`
   - Spectrometer name (spect): <spect>
   - Click ***Restore***
2. Restoring the backup file C:\Bruker\TOPSPIN\backup_old\nmr_backup.tar into the directory C:\Bruker\TOPSPIN\tmp:
   - Location of backup file: `C:\Bruker\TOPSPIN\backup_old`
   - Installation to be saved or restore destination: `C:\Bruker\TOPSPIN\tmp`
   - Spectrometer name (spect): <spect>
   - Click ***Restore***

If 'nmr_backup.tar' does not exist in the backup directory, the backup file 'xwin_backup.tar' will be taken (if existing)

After this process is finished, execute ***cf***.

8.8 Windows XP SP2 firewall configuration script

Microsoft Windows XP Service Pack 2 (SP2) includes significant changes to Windows networking functionality with regard to security aspects. After installation of SP2, Windows displays several informational dialogues about 'blocked components' and possible administrators activities during the start-up of TOPSPIN. Bruker BioSpin offers a configuration script '`setfirewall.cmd`' to apply the required settings to the new Windows XP SP 2 firewall.

Windows now includes fully featured firewall technology ('Windows Firewall', previously known as 'Internet Connection Firewall' or 'ICF'). After installation of SP2, the firewall is activated for all network interfaces by default, blocking network traffic to running applications that is initiated from external network locations. Bruker BioSpin's TopSpin software (as many other applications on the market) makes use of network connections for communication activities. Spectrometer control and TOPSPIN's 'remote connection' feature by design rely on network contacts from outside the local machine. As a result at start of TopSpin, Windows will bring up several information windows about 'blocked programs' recommending an administrator to review firewall settings to allow network communication for designated applications.

It is Microsoft's idea to have Administrators review for which applications network access from outside should be allowed. Those applications should be made 'known' to the firewall thus can be done manually using the '*Windows Firewall*' applet in the Control Panel.

Bruker BioSpin has developed a configuration script '*setfirewall.cmd*' that applies all required settings to Windows firewall configuration without user interaction. The script applies changes to the firewall related to Bruker software only and does not overwrite or reset entries for non-Bruker applications.

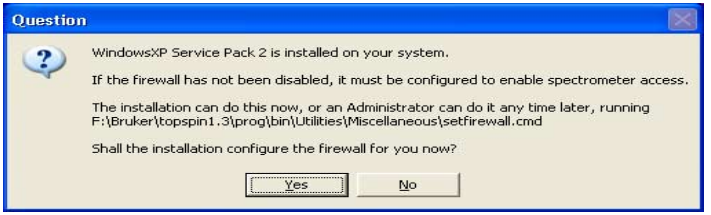
The script is stored in the subdirectory *<topspinhome>\prog\bin\utilities\Miscellaneous* of your TopSpin installation.

Note: If the script is executed in a wrong directory nothing will happen! Please note that the firewall is configured to allow 'Remote Connection' from local sub-

net addresses only

The script can be used in four different ways:

1. During the Installation of TOPSPIN (if the firewall is enabled) you will be asked to configure the firewall.


Question
WindowsXP Service Pack 2 is installed on your system.
If the firewall has not been disabled, it must be configured to enable spectrometer access.
The installation can do this now, or an Administrator can do it any time later, running F:\Bruker\topspin1.3\prog\bin\Utilities\Miscellaneous\setfirewall.cmd
Shall the installation configure the firewall for you now?
Yes
No

2. Click **Start** → **All Programs** → **Bruker TOPSPIN** → **Bruker TOPSPIN x.y** → **Bruker Utilities.** Double-click the script file: '*setfirewall.cmd*'. The script will automatically detect the installation path and register this installation with the firewall. I.e., if your installation were in '*F:\Bruker\ts13beta*' it would register that and only that!

   The script will automatically detect the installation path and register this installation with the firewall. I.e., if your installation were in '*F:\Bruker\ts13beta*' it would register that and only that!

3. Open the Windows Explorer and go to *<topspinhome>\prog\bin\utilities\Miscellaneous*. Double-click the script file: '*setfirewall.cmd*'.

   The script will automatically detect the installation path and register this installation with the firewall. I.e., if your installation were in '*F:\Bruker\ts13beta*' it would register that and only that!

4. Recommended for experienced administrators

   Copy the downloaded zip file to any location on your hard disk that does not contain '*prog\bin\utilities\Miscellaneous*' in its path. Execute it from a CMD prompt. You will get usage information like the following:

   `setfirewall INSTDIR SCOPE [DISKLESS_PATH [NFS_PATH]]`

   where

`INSTDIR`	installation directory of TOPSPIN, e.g. c:\Bruker\TOPSPIN
`SCOPE`	either ALL or SUBNET to specify whether firewall should allow remote connections to this installation from any address or local subnet only.

`DISKLESS_PATH`

installation directory of DISKLESS, e.g. c:\Bruker\Diskless

`NFS_PATH` installation directory of Hummingbird NFS Server, e.g.

`C:\Program Files\Hummingbird\Connectivity\7.10\NFSServer`

Note: You must have administrative rights to do this successfully

This way you have the possibility to register a specific installation of TOPSPIN with the firewall. Example:

`setfirewall f:\Bruker\ts12 ALL`

would do the required settings for an installation in '*f:\Bruker\ts12*' and allow the remote connection feature to be accessed without restrictions to the initiating network address. You can customize the script for different address ranges if required.

In case the installation path of Diskless or the NFS server is different from the default installation path, the script will inform you that the respective firewall configuration entries are not set. You have to execute the script manually and add the correct paths.

In either case, you should consider reexecution of the configuration script after one of the following actions happened:

- Complete reset of firewall settings (which is possible e.g. from Control Panel)
- TopSpin installation to new location
- Changes in Service Pack status (e.g. reinstallation)

For further questions and contributions, please feel free to contact software support at:

`nmr-software-support@bruker-biospin.de`

Chapter 9

User Management

9.1 User Management in a standalone PC

After the installation of Windows XP, there is one user with administrator rights, namely the user 'Administrator'. If the password for this user gets lost, there is no way of resetting it other than re-installing Windows XP. Therefore, we strongly recommend you install at least one more user with administrator rights, e.g. with the name 'root' (actually, this name is also much easier to type on the keyboard). You can install a new user or administrator as follows:

9.1.1 Adding a new user in a standalone PC (method 1)

The following chapter describes how to add a new user with Administrators rights:

1. Log in as Administrator
2. Click **Start** → **Control Panel** → **User Accounts**
3. A window '*UserAccounts*' will appear:
   - Click **Create a new account**
4. A window '*UserAccounts*' will appear
   - Enter the name of the new account e. g. **root** → **Next**
5. A window '*Pick an account*' will appear

- Click *Computer administrator* → **Create account**

Now you have created a new account. But this account is not protected by a password by default. Therefore you have to set a password for this account!

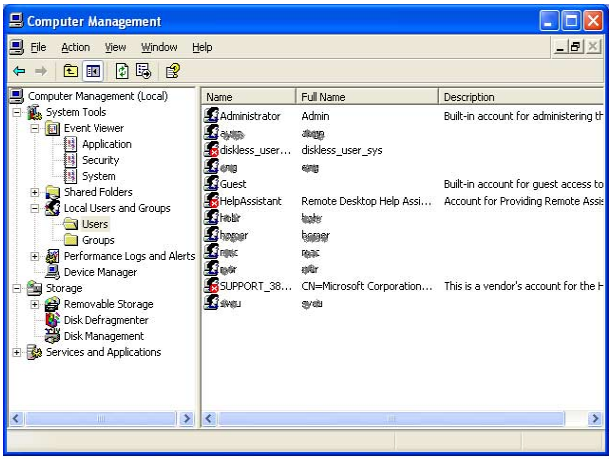
1. Click **Start** → **Control Panel** → **User Accounts**
2. A window '*UserAccounts*' will appear:
   - Click **Change an account**
   - Click the account you want to change → Click **Create a password**
   - Type in the password, confirm it and type in a password hint → **Create Password**

Now you have for example two users with local Administrator rights, Administrator and root. Whenever the password of one of them gets lost, you can login as the other one, open the User Manager and define a new password.

The creation of the new administrator account means that the user 'Administrator' is hidden in the log in menu. You are able to log in as the user 'Administrator' by pressing twice **Ctrl+Alt+Delete** in the log in window.

9.1.2 Adding a new user in a standalone PC (method 2)

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage** *or:* Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
2. A window *Computer Management* will appear:



- Click **Local Users and Groups**

3. Right mouse click **User** → Select **New User**
4. A window '*New User*' will appear
   - Enter the users **Full Name** and **Description** (optional) and the users password in the fields **Password** and **Confirm Password** → **Create** → **Close**

9.1.3 Adding normal users to the group NmrUser in a standalone PC

Each user who wants to run TOPSPIN must be a member of the group NmrUser. This group is automatically created during the TOPSPIN installation. To add a user, log in as Administrator (otherwise you will be asked for the administrator password during the process) and proceed as follows:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
   or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
2. A window *Computer Management* will appear:
   - Click **Local Users and Groups**
3. Click **Groups**
4. Highlight the group '**NmrUser**'
   - right mouse click → **Properties**
5. A window '*NmrUser Properties*' will appear:
   - Click **Add**
6. A window '*Select Users*' will appear:
   - Click **Advanced** → Click **Find Now**
   - highlight every name you want to be a member of NmrUsers
   - Click **OK** → **OK**
7. Close the window '*NmrUser Properties*' by clicking **OK**

or:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
   or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
2. A window *Computer Management* will appear:

- Click **Local Users and Groups**

3. Click **User**
4. Highlight the user '**root**'
   - right mouse click → **Properties**
5. A window '*root Properties*' will appear. Open the folder *Member of*.
   - Click **Add**
6. A window '*Select Groups*' will appear:
   - Click **Advanced** → Click **Find Now**
   - highlight group you want to be a member of
   - Click **OK** → **OK**
7. Close the window '*NmrUser Properties*' by clicking **OK**

9.2 User Management in a Domain PC

9.2.1 Adding a second user with Administrator rights in a domain PC

The group '*domain admins*' are automatically a member of the local group '*administrator*' so it is not necessary to create a second user with administrator rights.

9.2.2 Adding a local user in a domain PC

1. Log in as Administrator
2. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
   or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
3. A window *Computer Management* will appear:
   - Click **Local Users and Groups**
4. Highlight '*User*'
   - right mouse click → **New User**
5. A window '*New User*' will appear
   - Enter the users **Full Name** and **Description** (optional) and the users pass-

word in the fields **Password** and **Confirm Password** → **Create** → **Close**

6. Highlight the user you had just create
   - right mouse click **Properties**
7. A window '<*Username*> *Properties*' will appear:
   - Click **Member off** → **Add**
8. A window '*Select Groups*' will appear:
   - Click **Advanced** → Click **Find Now**
   - highlight every name you want to be a member of NmrUser
   - Click **OK** → **OK**
9. Close the window '<*Username*> *Properties*' by clicking **OK**

Click **Start** → **Shut Down**

Select **Log off Administrator**

Click **OK**

Press **CTRL+ALT+DEL**

→ Now you can log on as the new user

9.2.3 Adding normal users to the group NmrUser in a domain PC

Each user who wants to run TOPSPIN must be a member of the group NmrUser. This group is automatically created during the TOPSPIN installation.
To add a user, log in as Administrator (otherwise you will be asked for the administrator password during the process) and proceed as follows:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
   or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
2. A window *Computer Management* will appear:
3. Click **Local Users and Groups**
   - Click **Groups**
4. Highlight the group '***NmrUser***'
   - right mouse click → **Properties**

5. A window '*NmrUser Properties*' will appear:
   - Click **Add**
6. A window '*Select Groups*' will appear:
   - Click **Advanced** → Click **Find Now**
   - highlight every name or group you want to be a member of NmrUser
   - Click **OK** → **OK**
7. Close the window '<*Username*> *Properties*' by clicking **OK**

9.2.4 Adding a global group to the local group NmrUser in a domain PC

Users who want to use TOPSPIN must be member of the group NmrUser. In a Domain scenario we recommend to administrate users in global groups which are added to the local group NmrUser. Proceed as follows:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
   or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
2. A window *Computer Management* will appear:
3. Click **Local Users and Groups**
   - Click **Groups**
4. Highlight the group '**NmrUser**'
   - right mouse click → **Properties**
5. A window '*NmrUser Properties*' will appear:
   - Click **Add**
6. A window '*Select Users*' will appear:
   - Select in the field '*Location*' the domain name
   - In the window '*Enter Network Password*' type in your login name and password
   - Highlight the global group you want to be a member of NmrUsers (normally this is the group '*Domain Users*')
   - Click **OK** → **OK**
7. Close the window '*NmrUser Properties*' by clicking **OK**

Part II

Windows XP - Installation and Configuration

Chapter 10

Installation procedure

Before you start:

10.1 Do's and Don'ts under Windows XP

10.1.1 Do not re-install Windows XP

Not only will it usually not cure the problem, you also lose all additional pre-installed software (e.g. TOPSPIN, Office package, user accounting, screen and network drives etc.). YOU will have to put all of these back on manually. In such a case it is very important to have a backup of the essential files (see chapter 15.11 and 8.7). It will be many hours until you are back where you started. **If you have problems, use the Event Viewer and the other diagnostic tools to locate the problem and cure it within Windows XP.** If you think you need a re-install consider an 'Windows XP repair'. Use the Windows XP Repair diskettes (creating described in chapter 12) to repair Windows XP to the status of that repair disk rather than doing a scratch install. Re-installing Windows XP is a last resort and you should have very good reason to do it.

10.1.2 Use Windows sharing rather than FTP

Under Windows you locate other computers in the network with Windows Explorer and then you can use **drag-and-drop multiple files and entire directo-**

ries. You can also connect to UNIX machines in that fashion using a UNIX tool called 'samba'. Installation details are in chapter 13.4.3. Nevertheless, in some cases FTP is still the easiest way to get a file quickly.

10.2 Removing existing software

Windows XP is more complex than you might think. Many files that are uploaded during an installation go into other parts of the system or replace existing versions of files. Thus, an uninstall is more like a build-back and you need that to really clean things out. By removing the directory, you don't solve your problem and also you lose the installation log which is stored as the software is installed. This log is very important and used by the uninstaller to make sure it finds every file that went on in the first place.

Use the uninstaller from Control Panel, i. e. the icon labeled 'Add/Remove Programs'.

Without a log this software will not work any more. If the TOPSPIN is already installed and you want to install a new version or re-install the same version, you must first remove the old version and reboot the computer.

Your own AU programs, pulse programs and parameter sets are NOT removed when you de-install TOPSPIN. If you want to re-install any other package like NFS, you must first remove that package (see below), reboot the computer and then re-install the package.

Never delete directories to remove a program

Always use the 'Add/Remove Programs' tool

Re-install a program in the following way:

→ remove the program → reboot → install the program → reboot

1. Click **Start** → **Settings** → **Control Panel**
2. Double-click the icon **Add/Remove Programs**
3. A window '*Add/Remove Programs*' will appear:

   If you want to re-install the entire TOPSPIN (see chapter 6.4), please remove the packages:

   - Bruker: TOPSPIN
   - Bruker: AURELIA/AMIX

- Bruker: ICON-NMR
- Bruker: DISKLESS
- Bruker: NMR-SIM
- Bruker: TOPSPIN patches
- Bruker: SBASE
- Bruker: FLEXlm
- Bruker: NMR-GLP
- Bruker: NMR-GUIDE

Note that not all of these packages are necessarily installed!

a) Select the package that you want to remove

b) Click the button **Change/Remove**

c) A window '*Check Setup Information*' will appear

d) Check if the path is correct then click **OK**

e) A window '*Remove Programs From Your Computer*' will appear:

- A growing bar shows the progress of the de-installation
- When the de-installation is finished: click **OK**

f) Repeat step b) to e) to remove further packages or click **OK** to close the window '*Add/Remove Programs*'

4. Close the window '*Control Panel*'

5. Reboot the computer.

During the installation of the TOPSPIN, several entries are made in the Windows XP Registry. If an TOPSPIN package, e.g. TOPSPIN is removed as described above, the corresponding entry in the Registry is automatically deleted.

10.3 Autorun of installation programs

TOPSPIN (like many other software packages) support the Autorun feature. This means that the installation program automatically starts up when you insert the CDROM. This, however, only works if the Autorun is enabled. If it is not, nothing will happen after inserting the CDROM. In this case you can start the installation program as follows:

1. Click **Start** → **Control Panel**

2. Double-click the icon **Add/Remove Programs**

3. Click **Add New Programs** → **CD or Floppy**

4. A window '`Install Program from Floppy Disk or CD-ROM`' will appear:

The system is looking for a Floppy and/or a CD-ROM. If there are one of these the path will be shown in the field 'Open'

Click **Finish**

4a. If the field 'Open' is empty:

a) Click **Browse**

b) In the field 'Look in': select the CDROM drive

c) Find an icon **Setup** or **Setup.exe**

d) Click **Setup** or **Setup.exe**

or

1. Open the explorer (see 18.1.5)

2. Select the path of the CDROM drive (normally D:)

3. Double click on the file setup.exe

The Administrator can re-enable Autorun by changing the Registry entry

Warning: You are about to edit the Windows Registry File. This is Windows XP's nerve center and errors in your setup may render your Windows XP installation UNUSABLE. Please make sure you have a recent Windows XP Repair Disk created BEFORE you proceed.

HKEY_LOCAL_MACHINE\SYSTEM\CurrentControlSet\Services\Cdrom\Autorun

from 0 to 1.

Chapter 11

Installing and configuring Windows XP Professional

Windows XP exists in two different forms: Windows XP Professional and Windows XP Home Edition.
The installation as described in this chapter is valid for the English version of Windows XP Professional on a hp workstation xw4100. In this case, you can install Windows XP exactly as described here. For other versions of Windows XP or other hardware, the installation procedure might be different.
For example, on some PC's the boot sequence is interrupted with the **Delete** key rather than with the **F2** key.

This description is intended for new installations. If Windows XP is already installed and you have problems:

!

Before you decide to re-install Windows XP, try to repair Windows XP

Repairing Windows XP means that you selectively re-install parts of Windows XP, leaving application software and data intact.

11.1 Scratch install of Windows XP

1. If your computer is running:

a) Click **Start** → **Shut Down** → **Shut down the computer** → **Yes**

b) When you see the text '`It is safe to turn off your computer`' insert the CD-ROM '*Windows XP Professional*'.

2. Restart the computer and **Interrupt** the boot process by pressing the **F8** key.

(Do not press **F2** to go into *BIOS*, because there you can easily make your PC unable to boot.)

3. Wait until the boot device menu appears, select removable device with the **ARROW KEY DOWN** → **ENTER**

4. The '*Windows Setup*' screen appears:

a) You see at the bottom of the window '*Setup is loading files*'.

b) You see at the bottom of the window '*Setup is starting Windows XP*'.

5. A '*Windows XP Professional Setup - Welcome to Setup*' screen will appear with the Option of Continuing Setup, Repair a previous installation, or Quitting:

a) Press **ENTER** to Continue Setup.

6. A text about the "Windows XP Licensing Agreement" (EULA) screen will appear:

- Press the **PGDN** key repeatedly until the end, press **F8** (to accept).

  You see at the bottom of the window '*Searching for previous versions of Microsoft Windows*'.

7. If you have already other Windows XP installations on your PC, a list of them will appear. Press ESC in order to make a new installation instead of repairing an older one

8. If you have a couple of partitions on your hard disk, a list of currently available partitions will appear:

a) Press the **ARROW UP** or **DOWN** key to highlight the partition on which Windows XP must be installed.

!

b) Press **ENTER**

- Select **Format the partition using the NTFS file system**, press **ENTER**

! You are asked if you really want to format this partition or want to choose a different partition. After this point formatting will be started, ALL DATA ON THIS PARTITION WILL BE LOST! Data on other partitions (which might be on the same disk) remain untouched. If you want to format this partition, press **F** (to start formatting) and wait...

9. A window '*Your Computer will reboot in 15 s*' will appear

Remove any Floppy but keep the CD in its drive.

10. After the reboot the setup will continue automatically

A window '*Windows XP Setup*' occurs, please wait ...

11. A window '*Windows XP Professional Setup*' will appear:

a) Click **NEXT** or wait for a short time

b) Installing Devices (wait ...)

c) '*Regional Settings*'

- Normally you could leave English (United States) for system locale. Set the right keyboard layout → **NEXT**

d) '*Personalize Your Software*'

- Type in your name and organization → **NEXT**

e) '*Your Product Key*' (see list in chapter 21.1):

- Enter the **Product ID** which is specified on the manual '*Microsoft Windows XP Professional*' (on the Certificate of Authenticity) → **NEXT**

f) '*Computer Name and Administrator Password*' (see list in chapter 21.1):

- Enter the **Name** (hostname) you have chosen for your computer

  Note that the first character must be alphanumeric and underscores are not allowed

- Choose an Administrator password and enter it in the field **Password**, enter the same password in the field **Confirm Password**→ **NEXT**

! Important: remember the Administrator password.

g) '*Date and Time Settings*'

- Check if Date&Time are set correctly, change if necessary

  Select the correct time zone for your location, e.g.:

`GMT + 01:00` for Germany
`GMT - 05:00` for the US east coast
`GMT - 08:00` for the US west coast

- click **NEXT**

h) '*Networking Settings*' (wait ...)

- Enable Typical Settings→ **NEXT**

i) '*Workgroup or Computer Domain*'

- To get this information contact your system administrator, if you are not sure at the moment, please choose '*No, this computer is not on a network ...*' and enter the workgroup name → **NEXT**, please wait ...

j) The text '*Performing Final Tasks*' appears:

- please wait ...

k) The text '*Completing the Windows XP Setup Wizard*' appears:

- click **FINISH**, the system will reboot

l) Eject the CD-ROM

12. A window '*Network Identification*' will appear → **NEXT**

a) Users of this computer - who can log on to this computer?

- Enable '*Users must enter a user name ...*', click **NEXT** → **FINISH**

You can log in as Administrator using the password which you have entered during the installation.

11.2 Installing Windows XP Service Pack

PCs from Bruker Biospin are delivered with the latest Service Pack available at the time of delivery. Under Windows XP it is not necessary to reinstall the service pack after e. g. configuring the network.

The Service Pack can be downloaded from `www.microsoft.com` or `www.microsoft.de`.

For installation just follow the given instructions on the screen.

11.3 Installing the Graphics driver

Hewlett Packard PCs from Bruker BioSpin are delivered with the Graphics driver on the CD. If you do not have a floppy or a CD and want to install a newer driver, you can download a Graphics driver from the Web. Go to:

`http://h20000.www2.hp.com/bizsupport/TechSupport/Product.jsp?prodTypeId=12454&prodCatId=296720&locale=en_US&taskId=135`

The Graphics drivers are offered as self-extracting `.exe` files. Just download the file for your system, then click its icon and insert a formatted floppy. This way, you can create a new Graphics driver floppy.

The Graphics driver CD can be installed as follows:

1. Insert the Graphics driver CD
2. Click **Start** → **Control Panel**
3. A window '*Control Panel*' will appear:
   - Double-click the icon **Display**
4. A window '*Display Properties*' will appear:
   - Click **Settings**
5. If the window 'Invalid Display Settings' appears: click **OK**
6. Click **Advanced** → **Adapter** → **Properties** → **Driver** → **Update Driver**→ **Next** → enable **'Display a List ...'** → **Have Disk**
7. A window '*Install From Disk*' will appear:

   Enter your CDROM, e.g. **d:** or accept the default if it is correct → Click **OK**
8. The Graphics driver which resides on the CDROM will appear: Click **OK**
9. A window '*Third-party Drivers*' will appear:
   - Click **Yes** (to proceed) and wait ...
10. A window '*Installing Driver*' will appear: click **OK**
11. In the window '*Upgrade Device Driver Wizard*': click **Finish**
12. Close the windows you have just opened
13. Remove the CD
14. A window '*Systems Settings Change*' will appear: click **Yes** (to reboot)

The procedure for other PC's or other Graphics drivers might be a little different.

Chapter 12

Configuring Windows XP

12.1 Conversion of disk format from FAT to NTFS

Windows XP supports three file systems for disks: FAT16, FAT32, and NTFS.

Bruker BioSpin TOPSPIN and the datasets of the NMR experiments requires the file format NTFS. So if you use a FAT-partition of your harddisk(s), you have to convert this partition to 'NTFS' (that is the file system of Windows XP) before you can install the TOPSPIN. Only under NTFS, it is possible to have the file permissions, ownership and access management settings that make Windows XP secure. You can use the convert command `convert.exe` to convert an existing FAT volume to NTFS. Because this conversion retains all of your files, use `convert.exe` when you want to keep existing files on your volumes intact.

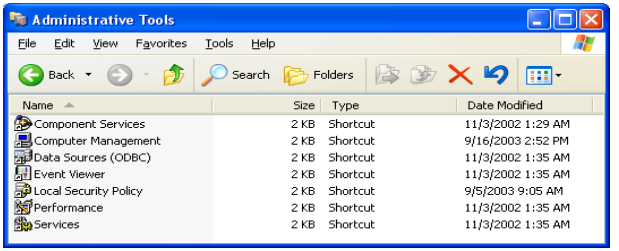
The conversion to NTFS is a one-way process. After you convert a drive or partition to NTFS, you cannot convert it back to FAT. To restore the volume to the previous file system, you must format it as FAT again. This action erases all existing data including your programs and personal files. In this case, you must either restore your data from a backup, or reinstall your operating system and programs.

`convert.exe` requires that you have a certain amount of free space on the drive or partition to convert it. If `convert.exe` determines that there is not enough free space on the volume, it does not convert the volume.

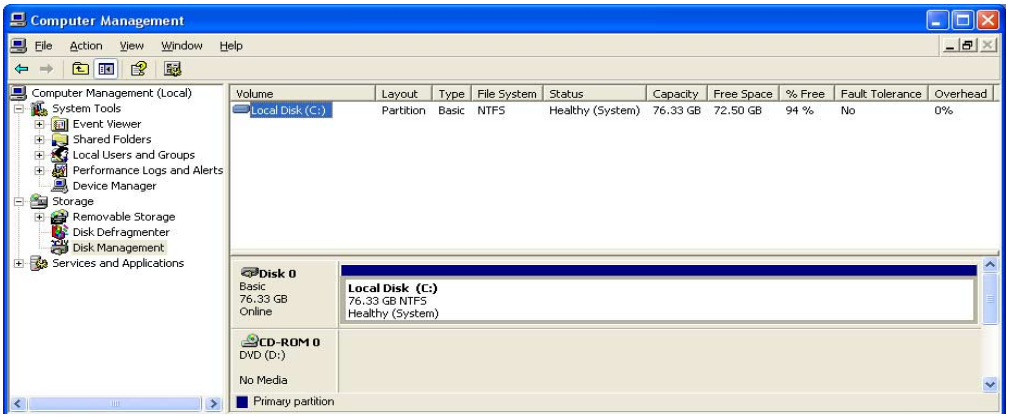
12.1.1 Check the Disk Partitioning

To check the configuration of the disk(s) of your PC, please start up the Disk Administrator utility from the command menus as shown below:

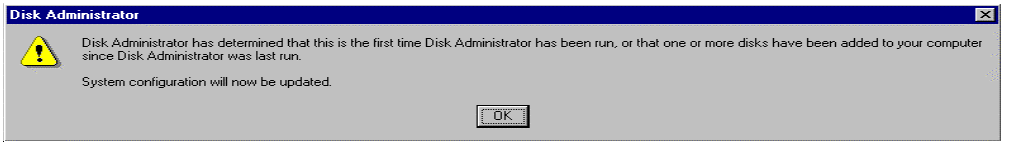
1. Click **Start → Control Panel → Administrative Tools**

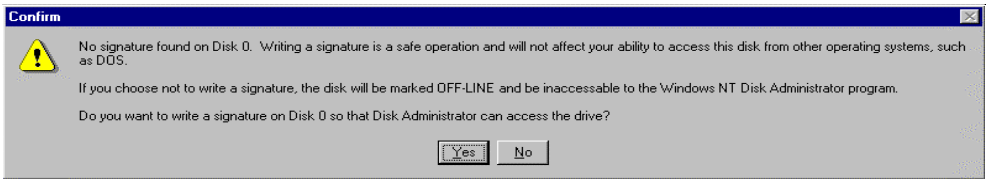

Administrative Tools
File Edit View Favorites Tools Help
Back Search Folders
Name Size Type Date Modified
Component Services 2 KB Shortcut 11/3/2002 1:29 AM
Computer Management 2 KB Shortcut 9/16/2003 2:52 PM
Data Sources (ODBC) 2 KB Shortcut 11/3/2002 1:35 AM
Event Viewer 2 KB Shortcut 11/3/2002 1:35 AM
Local Security Policy 2 KB Shortcut 9/5/2003 9:05 AM
Performance 2 KB Shortcut 11/3/2002 1:35 AM
Services 2 KB Shortcut 11/3/2002 1:35 AM

2. Click on **Computer Management → Disk Management**



If this is the first time you start Disk Administrator, you probably see two information screens which you can confirm by clicking **OK,** respectively **Yes**:


Disk Administrator
Disk Administrator has determined that this is the first time Disk Administrator has been run, or that one or more disks have been added to your computer since Disk Administrator was last run.
System configuration will now be updated.
OK


Confirm
No signature found on Disk 0. Writing a signature is a safe operation and will not affect your ability to access this disk from other operating systems, such as DOS.
If you choose not to write a signature, the disk will be marked OFF-LINE and be inaccessable to the Windows NT Disk Administrator program.
Do you want to write a signature on Disk 0 so that Disk Administrator can access the drive?
Yes No

Finally, the disk administrator will show you how many disk drives your system has, and how they are partitioned.

Please realize that repartitioning the C: partition involves re-installing Windows XP!

Also, the maximum partition size with FAT is 4 GByte, with NTFS 7.8 GByte. Nevertheless, if you decide to make changes in the partitioning now is a good time to do it because you did not invest too much time in configuration and installation yet (e. g. the TOPSPIN is not installed and configured so far). All other partitions are usually empty at delivery of the PC and you can re-partition them or assign different drive letters. An other file system format is FAT32 that has the advanced of none maximum partition size and that could be read by windows 9x, NT and 2000.

12.1.2 Converting partitions from FAT to NTFS

You see that in our case, both C: and D: already have the NTFS file system. If, on your system, partition D: or any other partition on which you want to store NMR data is FAT, you can change that from the Disk Administrator. Just click

All Tasks → **Format** from the **Action** menu, select the NTFS file system and Start formatting.

Be aware that this will erase the entire partition.

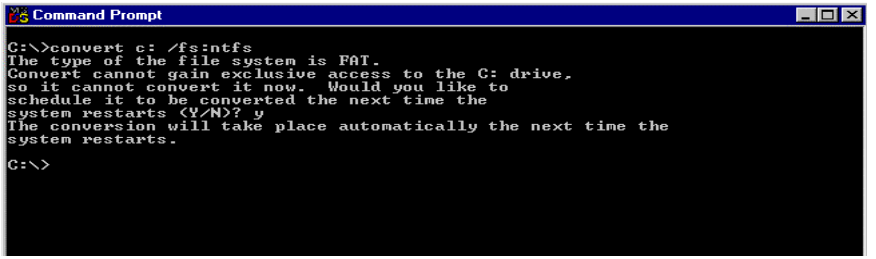
The C: drive cannot be converted from the disk administrator. It can, however, be scheduled for conversion during the next boot up. In this way, the entire contents of C:, like Windows XP, will remain intact. Important: This is again a critical operation concerning power loss. If the conversion runs and the power goes away it will render the disk unusable and Windows XP must be re-installed. So it might be a good idea your PC to connect to an Uninterrupted Power Supply before you move on.

To convert a drive from FAT to NTFS without loss of data, start a Command Prompt from the command menus: Then type the following command on the command line and press return:

```
convert <drive:> /fs:ntfs
```

The system will ask you to schedule the actual conversion for the next boot-up and

you will reply with '**y**' as shown below:


Command Prompt
C:\>convert c: /fs:ntfs
The type of the file system is FAT.
Convert cannot gain exclusive access to the C: drive,
so it cannot convert it now. Would you like to
schedule it to be converted the next time the
system restarts (Y/N)? y
The conversion will take place automatically the next time the
system restarts.
C:\>

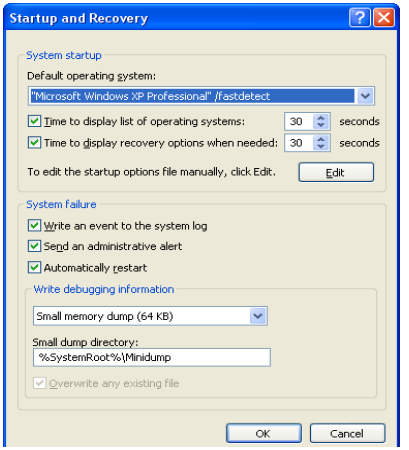
you do NOT need to re-boot now and wait the 2-3 minutes for it to complete. Just move on with the operations explained in the next chapter. The conversion to NTFS will automatically be done during the next re-boot.

12.1.3 Cutting down the re-boot time

1. Click **Start** → **Control Panel** → double click on **System**

   A window '*System Properties*' will appear:

2. Click **Advanced** → **Startup and Recovery**:



The default entry for the time the system waits for your boot selection during boot up is set to 30 seconds. You can set this entry to 5 seconds which is usually enough to select a different boot mode (or partition) if you want to do that.

3. Click **OK**

Chapter 13

Windows XP Networking

! In order to run TOPSPIN, you must setup the network (TCP/IP protocol), even if your PC is not connected to a spectrometer or to the laboratory network.[1] You can setup the network as a so-called Domain scenario or as Workgroup scenario. This chapter describes the Workgroup scenario.

13.1 TCP/IP configuration

This chapter describes how to install both the laboratory network (Workgroup scenario) and the spectrometer internal network for a 'hp workstation xw4100'. The description for other PC's with a different Ethernet card might be a little different. Before you start, make sure all network hardware components (network card, adapter, cables etc.) are properly connected. Then make a list of the following information:

- IP address for the PC in the laboratory network
- subnet mask of the laboratory network
- DNS domainname of the laboratory network
- IP address of the DNS nameserver(s) (if a nameserver exists)

1. The TOPSPIN license requires TCP/IP to be installed.

- IP address of the default gateway (if a default gateway exists)

If your PC is not physically connected to the laboratory network, you can use any IP address, subnet mask and domainname for the (external) network configuration. A frequently used IP address for such a 'standalone' computer is 192.168.0.1. This address is not assigned to any network computer (by world-wide-agreement). However, for the spectrometer internal network, you must use the values as specified below.

Perform the following steps according to the necessities of your setup:

13.1.1 Create a New Network Connection

1. Log in as Administrator
2. Click **Start** → **Control Panel** → **Network Connections**
3. A window *Network Connections* will appear
4. Click on *Create a new connection* on the left side of the window
5. A window *Network Connection Wizard* will appear → **NEXT**
6. Enable *Connect to the Internet* → **NEXT**
7. A window *Now Getting Ready* will appear
8. Enable **Connect using a broadband connection that is always on** → **NEXT**
9. A window *Completing the New Connection Wizard* will appear → Click **FINISH**

13.1.2 Configuring the TCP/IP of an existing Network Connection

1. Log in as Administrator
2. Click **Start** → **Control Panel** → **Network Connections**
3. A window '*Network Connections***'** will appear
4. Highlight the connection you want to configure → **File** → **Properties**
5. Highlight the TCP/IP entry and click **Properties**
6. The window '*Internet Protocol (TCP/IP) Properties*' will appear:
7. Enable '*Use the following IP address*'

   b) In the field **IP Address**: enter the IP address of your computer

   c) In the field **Subnet Mask**: enter the subnet mask of your network

e.g. 255.255.255.0 or 255.255.0.0

d) In the field **Default Gateway**: enter the IP address of the Default Gateway in your network (if available)

e) If you have a nameserver:

- In the field **Prefered DNS Server** enter the IP address of the nameserver
- If you have a second nameserver enter his IP address in the field *'Alternate DNS server'*

f) Click **Advanced → DNS**

g) Enable the field **Append these DNS suffixes (in order) → Add**

- In the window *'TCP/IP Domain Suffix*':

  Enter the network domainname **→ Add**

h) Click **OK**

i) If the question appears:

'This connection has an empty primary WINS address. Do you want to continue?' **→ YES → OK → OK → CLOSE**

13.1.3 Configuring the TCP/IP of the Spectrometer Control:

1. Log in as Administrator

2. Click **Start → Control Panel → Network Connections**

3. A window *'Network Connections***'** will appear

4. Highlight the connection you want to configure **→ File → Properties**

5. Highlight the TCP/IP entry and click **Properties**

6. The window *'Internet Protocol (TCP/IP) Properties*' will appear:

- In the field **IP Address**: enter **149.236.99.1**
- In the field **Subnet Mask**: enter **255.255.255.0**

! For the spectrometer network ONLY THESE VALUES ARE VALID!

Do not choose different settings for the IP address or Subnet mask.

- Leave the Field Default Gateway empty

7. Click **OK**

If your PC controls a spectrometer we recommend to do the following:

1. Click **Start** → **Control Panel** → **Network Connections**
2. A window '*Network Connections*' will appear:
   a) Select the Adaptor to which the spectrometer CCU is connected. This is normally, but not necessarily Adaptor 2.
   b) Right mouse click → **Properties**
   c) Disable the entry **Client for Microsoft Network (TCP/IP) by** clicking on the '**+**' sign to the left of the entry

13.2 Changing the hostname of the computer and its effects

If you want to change the hostname of your PC you can do this in the following way. IMPORTANT: You also have to change the text-file:

`<TOPSPINHOME>\conf\nmrsuperuser`

This file contains the computer-name and the Windows XP user which is the TOPSPIN-SUPERUSER. You can edit and change this file with a normal text editor like notepad if you are logged in as the Windows XP-user which is the NMRSUPERUSER.

1. Log in as Administrator
2. Click **Start** → **Control Panel** → **Network Connections**
3. A window '*Network Connections*' will appear:
   a) Click **Advanced** → **Network Identification**
   b) A window '*System Properties*' will appear
   c) Click **Network Identification** → **Properties**
   d) In the field **Computer Name**: enter the new hostname

Note that the first character must be alphanumeric and underscores are not allowed!

   e) Click **OK**
4. A window '*Network Identification*' will appear:
   - Click **OK**
5. In the window '*System Properties*':

- Click **Close**

6. A window '*System Setting Change*' will appear:

- Answer the question if you want to restart the computer now by clicking **Yes**

7. If you have *Floating* licenses you must change the hostname in the file `license.dat`. By default it resides in `C:\flexlm\Bruker\licenses`. You can do this in the following way:

a) Click **Start** → **All Programs** → **Accessories** → **Command Prompt**

b) Enter: **`cd c:\flexlm\Bruker\licenses`**

c) Enter: **`notepad license.dat`**

- Change the hostname in the SERVER line, then save and exit the file.

Of course, you can also change the license file from the Explorer. We have chosen the Command Prompt because the Explorer might add the (hidden) extension `.txt` to the file `license.dat` which makes it unusable (see chapter 16.1.3).

13.3 Network diagnostic commands

Here is a list of the most important network diagnostic commands as they can be entered from the Command Prompt:

- **`arp`** - displays or modifies the IP to physical address translation tables
- **`hostname`** - displays the name of the current host
- **`ipconfig`** - displays information about the current TCP/IP configuration
- **`netstat`** - displays protocol statistics and current TCP/IP connections
- **`ping`** - checks if a destination host is receiving TCP/IP packets
- **`route`** - maintains and displays routing tables
- **`tracert`** - displays the route packets take to a destination host
- **`net start`** - displays all running services
- **`net use`** - display current network connection
- **`nbtstat -a`** - displays all registered NetBIOS names

13.4 Accessing remote files and directories

13.4.1 Sharing directories from a Windows XP host

Network operations under Windows XP primarily takes place via the Windows XP sharing mechanism. For example, you can share the data directory `c:\data` on *nthost_a* by taking the following steps:

1. Log in as Administrator on *nthost_a*

2. Open drive `C:` in the Explorer

3. Right-click on **data**

4. A popup window will appear:

Click **Sharing and Security**

5. A window '*Data Properties*' will appear:

a) Click **Share this folder**

- Accept the default shared name *data*, or enter any other name [1]
- Optionally, you can enter a comment

b) Optionally, you can set a user limit and/or shared permissions (note that the default permissions are Full Control for Everyone)

c) Click **OK**

The directory `c:\data` can now be accessed from any Windows XP host in the network, e.g. from *nthost_b*, in the following way:

1. Log in on *nthost_b* as normal user

2. Click the icon **My Network Places** on the desktop

3. A list of hosts in the network will appear:

- Double-click the icon of *nthost_a*

4. A window '*Enter Network Password*' will appear:

a) In the field **Connect As**: enter the name of any user on *nthost_a*

b) In the field **Password**: enter the password for this user

→ A list of shared partitions/directories will appear

1. This is the name under which the directory can be accessed from other hosts

(The network password is only requested for the first connection).

Now you can:

- Access the remote directory as if it were local
- Copy the remote directory or any sub-directory or file in it, by dragging the corresponding icon into any target directory window (assuming you have the write permission in the target directory).

Note that the latter is only useful if the remote directory is not permanently shared.

13.4.2 Enabling and disabling Simple File Sharing

A PC under Windows XP Professional that is joined to a workgroup has the Simple File Sharing enabled by default. The Simple File Sharing is located in the folder's properties. When you set the Simple File Sharing the share and the file permissions are configured.

A Windows XP Professional PC that is joined to a domain use only the classic file sharing and security interface.

If you disable Simple File Sharing, the Shared Documents feature is not turned off.

You have more control over the permissions to individual users, if you disable the Simple File Sharing, However, you must have advanced knowledge of NTFS and share permissions to keep your folders and files secure.

! It is recommended that you share folders only on the network within your user profile that remote users on other computers need to access. Never ever share the root of your system drive. In this case your computer is more vulnerable to malicious remote users.

To turn Simple File Sharing on or off:

1. Double-click **My Computer** on the desktop.
2. Click on **Tools**, select **Folder Options**.
3. Click the **View** tab, then click to clear the **Use Simple File Sharing (recommended)** check box to disable Simple File Sharing.
4. Click **OK**.

Levels of Access

There are five levels of access:

1. Level 1: My Documents (Private)
2. Level 2: My Documents (Default)
3. Level 3: Files in shared documents available to local users
4. Level 4: Shared Files on the Network (Readable by Everyone)
5. Level 5: Shared Files on the Network (Readable and Writable by Everyone)

In Levels 1, 2, and 3 folders are available only to a user who is logging on locally. Levels 4 and 5 folders are available to users who log on locally and remote users from the network .

You can have the following permissions:

Access Level	Everyone (NTFS/File)	Owner	System	Administrators	Everyone (Share)
Level 1	no	Full Control	Full Control	no	no
Level 2	no	Full Control	Full Control	Full Control	no
Level 3	Read	Full Control	Full Control	Full Control	no
Level 4	Read	Full Control	Full Control	Full Control	Read
Level 5	Change	Full Control	Full Control	Full Control	Full Control

1. Level 1: My Documents (Private)

   Only the owner of the file or folder has the permission to read and write to the file or folder. All subfolders that are contained within a folder that is marked as private remain private unless you change the parent folder permissions. The option to make a folder private is only available to a user account in its own *My Documents* folder.

To Configure a folder and all of the files in it to Level 1:

a) Right-click the folder → click **Sharing and Security**.

b) Click to select the **Make this Folder Private** check box → click **OK**.

2. Level 2 (Default): My Documents (Default)

Only the owner of the file/folder and a local administrator have the permission to read and write to the file/folder. This is the default setting for all of the folders and files in each user's *My Documents* folder.

To configure a folder and all of the files in it to Level 2:

a) Right-click the folder → click **Sharing and Security**.

b) Ensure that both the **Make this Folder Private** and the **Share this folder on the network** check boxes are cleared → click **OK**.

3. Level 3: Files in Shared Documents Available to Local Users

Files are shared with users who log on to the computer locally. Local administrators and Power Users can read, write, and delete the files in the Shared Documents folder. Restricted Users can only read the files in this folder. In order to allow Remote Users to access folders/files at Level 3, you must share them out on the network (Level 4 or 5).

To configure a file/folder and all of the files in it to Level 3:

a) Start Microsoft Windows Explorer

b) Copy or move the file/folder to the Shared Documents folder under My Computer.

4. Level 4: Shared on the Network (Read Only)

For everyone on the network and local users (including the Guest account (if activated)) the files are shared to read. But they are not allowed to modify the contents. User that can connect to the computer on the network are able to read and change these files.

To configure a folder and all of the files in it to Level 4:

a) Right-click the folder → click **Sharing and Security**.

b) Click to select the **Share this folder on the network** check box

c) Click to clear the **Allow network users to change my files** check box → click **OK**.

5. Level 5: Shared on the Network (Read and Write)

   This level is recommended only for a closed protected network that has a firewall configured.

   This level is the most available and least secure of all access levels. Any user can read, write, change, or delete a file in a folder shared at this access level.

   To configure a folder and all of the files in it to Level 5:

   a) Right-click the folder → click **Sharing and Security**

   b) Click to select the **Share this folder on the network** check box → click **OK**.

NOTE: All NTFS permissions that refer to Everyone include the Guest account.

13.4.3 Sharing directories from a UNIX host using Samba

If you are logged in on a Windows XP host, you can access data which reside on a UNIX host, using the sharing mechanism. This, however, only works if the Samba package is installed on the UNIX host. Samba is available from http://www.samba.org/samba/download.html. Proceed as follows:

1. Download the correct version `samba53.*` or `samba6x.*` depending on your IRIX version (uname -r).
2. Install with **`inst -f sambaxx.2.0.xx.tardist`**
3. Within **`inst`** use **`list`** to show information about the package and **`go`** to install it.
4. After installation is done, you may configure it with the SWAT tool. This tool (Samba Web Administration Tool) is started, if you enter the address "http://localhost:901/" into your Web Browser. eg: **Toolchest** → **Internet** → **Open Web Browser**.
   - define the **workgroup** in the **GLOBALS** section
   - the **directories** you want to share in the **SHARES** section
   - and the password encryption settings. The default is **no** (see chapter 20.5.3), but Windows XP is sending encrypted passwords by default so you have to change it in Samba or in Windows XP (see step 7)
5. You will find an actual describtion of the current samba version and the corresponding installation in:

   `ftp://ftp.bruker.de/pub/nmr/binaries.indy/samba-x.readme`

More information on setting up `samba`, password encryption and many other features of Samba can be found in:

`/usr/samba/docs`

6. Reboot the UNIX host
7. If the `Samba` on the UNIX host is configured as '`encrypt passwords = no`' (check it in the SWAT) and you want this configuration, you must enable plain passwords on your PC. You could do that as follows *but be aware that this would create a security leak (see chapter 20.5.3)*:
   a) Log in as Administrator
   b) Get the file:

      `/usr/samba/docs/WinXP_PlainPassword.reg`

      from the UNIX host, e.g. with FTP
   c) Execute this file by clicking on its icon in the Explorer
   d) Reboot the PC

13.4.4 Mounting Windows XP partitions from a UNIX host using NFS

If your PC is controlling a spectrometer, installation of the Hummingbird NFS Server is mandatory. The partition `C:\Bruker\Diskless\clients\spect` is mounted via NFS by the spectrometer CCU (which is a UNIX host). In the same way, you can mount any Windows XP partition or directory on any UNIX host. Proceed as follows:

1. Export the Windows XP partition as described in chapter 6.6.1. In step 4, you must enter the partition and, optionally, the UNIX host(s) to which it must be exported.
2. On the UNIX host:
   a) Open a UNIX shell
   b) Type **`su`** to become superuser
   c) Create a mount directory, e.g. **`mkdir /ntdata`**
   d) mount the partition, e.g.:
      - on SGI: **`mount nthost:/c/data /ntdata`**
      - on X32: **`mount -f NFS nthost:/c/data /ntdata`**

      Note that, if the pathname on the Windows XP hosts contains uppercase let-

ters, these must also be specified with the mount command.

13.4.5 FTP

Network transfer under Windows XP is generally done via the directory sharing as described in chapter 13.4.1 and 13.4.3. Nevertheless, Windows XP supports transfer via FTP. Just enter '**`ftp hostname`**' from a Command Prompt and you can transfer files.

13.4.6 Telnet

Windows XP contains a **`telnet`** command for remote login. Just enter **`telnet hostname`** in a Command Prompt to login to a remote host. The telnet command can only be used to login from your PC to a remote host (e.g. a UNIX host) but not vice versa.

With Windows XP it is also possible to do a telnet login to a Windows XP computer but this feature is not very convenient.

13.5 Requirements for the 'Send' function in TOPSPIN

Alternatively to printing and faxing diagnostics results to Bruker BioSpin or somewhere else, you can send the same information via electronic mail. For this to work, the spectrometer PC needs access to the Internet, i.e. to an Internet gateway in your local network. If the Personal Computer has not yet been set up for e-mail transmission proceed as follows:

Install a program that allows for composing and sending e-mail messages. If you have **Microsoft Internet Explorer 6.0** or newer, we recommend to install it. Internet Explorer is bundled with an e-mail application called **Outlook Express.** Outlook Express is perfect for TOPSPIN's e-mail features.

The descripton how to use the send button in TOPSPIN or Xwin-nmr is found in the *TOPSPIN Processing Reference Manual.*

13.5.1 Installation and configuration of Outlook Express

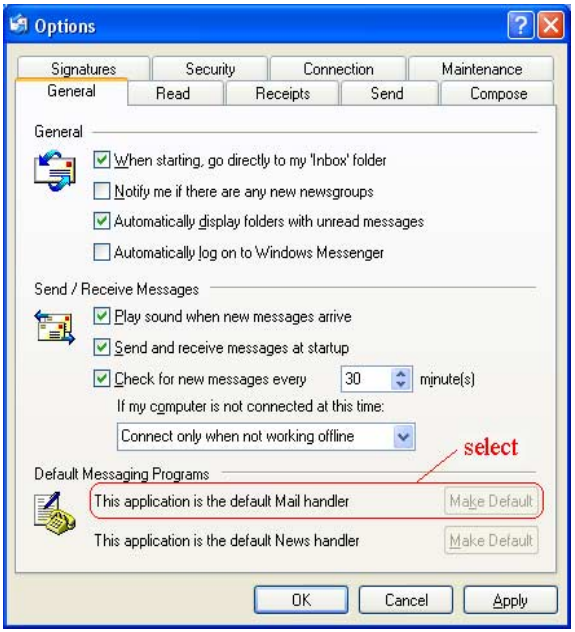
Outlook Express gets automatically installed with Microsoft Internet Explorer 6.0 or newer.

- Open **Start → All Programs →Outlook Express**

- or double-click the **Outlook Express** icon on the desktop.

Supply all parameters asked for by the setup wizard. Contact your network administrator if you are not sure what to fill in.

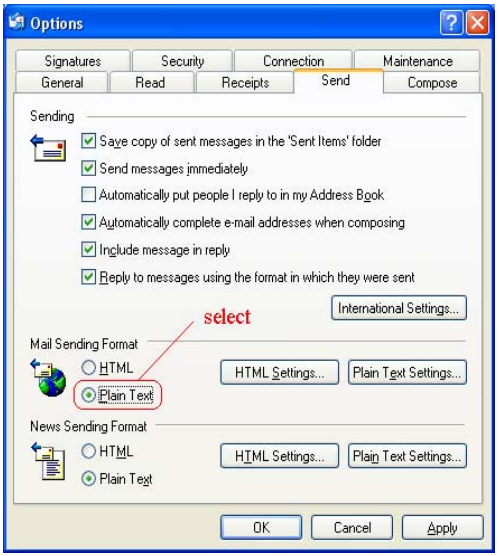
Select **Options** from Outlook Express' **Tools** menu and configure the General Settings as shown below.



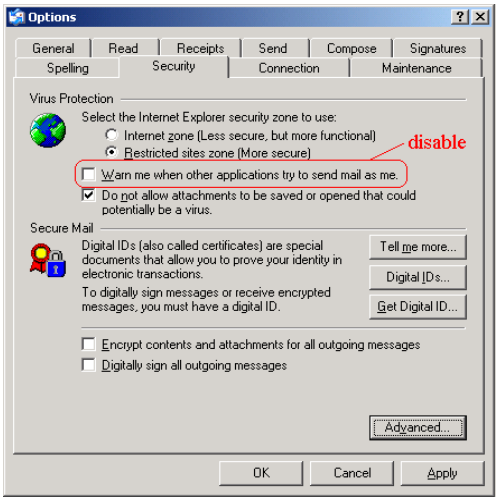
Outlook Express version 6 is able to handle the default mail handling and the simple MAPI client as one. It is sufficient to enable the setting as default mail program

Do not reboot the computer now. Open the **Options** interface again, switch to the

Send page and select the topics as shown below.



Switch to the **Security** page and disable *Warn me when other applications try to send mail as me*, then reboot the computer.


Options
General
Read
Receipts
Send
Compose
Signatures
Spelling
Security
Connection
Maintenance
Virus Protection
Select the Internet Explorer security zone to use:
Internet zone (Less secure, but more functional)
Restricted sites zone (More secure)
disable
Warn me when other applications try to send mail as me.
Do not allow attachments to be saved or opened that could potentially be a virus.
Secure Mail
Digital IDs (also called certificates) are special documents that allow you to prove your identity in electronic transactions.
To digitally sign messages or receive encrypted messages, you must have a digital ID.
Tell me more...
Digital IDs...
Get Digital ID...
Encrypt contents and attachments for all outgoing messages
Digitally sign all outgoing messages
Advanced...
OK
Cancel
Apply

To disable this warning might be a security leck. If you do not disable this warning, you get a warning every time if ICON-NMR send an e-mail.

13.5.2 Sending an e-mail with Outlook Express

- Fill in the correct recipient's address.
- Click the **Send** button.

If you want to use an e-mail application not mentioned here, make sure it has some 'use as simple MAPI client' feature and activate it.

13.6 Installing the TOPSPIN in a Windows XP Domain

Windows XP provides two different security scenarios for computer networks, the Workgroup and the Domain scenario. With a Workgroup scenario, each computer has its own local security database of user accounts and passwords. This means that users from workstation A are not known at workstation B. They might have the same name on both workstations but internally they are represented by two different security identifiers. Users from workstation A can access files on workstation B via the sharing mechanism (see chapter 13.4.1). The Workgroup scenario is typically used for small networks. For large networks, the Domain scenario is usually preferred. In this case, one computer (the Domain Controller, DC) maintains the security database for an entire group of Windows XP Computers. A Domain user can log on at each workstation in the Domain with a single account and password. Furthermore, the Domain Administrator's account has administration rights on every computer in the Domain. Nevertheless, a local Administrator account exists on each computer for local administration tasks.

Bruker BioSpin TOPSPIN fully supports both security scenarios. The description of the TOPSPIN installation in chapter 6.4 is valid for a Workgroup scenario. This chapter describes the additional installation steps which are required for a Domain scenario. The NMR Superuser (see chapter), which is specified during the installation of TOPSPIN can now be a local account or a Domain account. In both cases the NMR Superuser only needs standard access permissions. The installation of TOPSPIN, however, requires Administrator rights because certain system services and two user groups are installed. Furthermore:

TOPSPIN must be installed as local Administrator

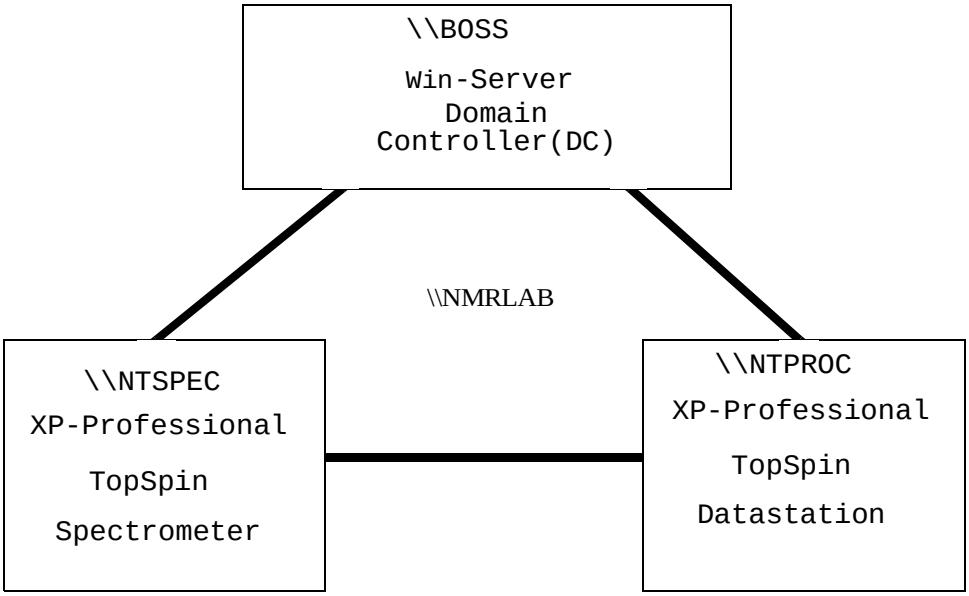
This means no Domain-wide administrative tasks are done during the installation. The installation of TOPSPIN in a Domain involves the following steps:

1. Make sure that there is a Local or Domain account for NMR Superuser, or cre-

ate one.

2. Installation of TOPSPIN by the local Administrator.
3. Creation and configuration of global groups of NMR users by the Domain Administrator.
4. Make sure that all nmr users have an existing HOME directory

As an example, we use a Domain *\\NMRLAB* with two workstations; *\\NTSPEC* which controls a spectrometer and *\\NTPROC* which is used for processing. The security database resides on the Domain Controller *\\BOSS*. Step 2, the installation of TOPSPIN is the same on *\\NTSPECT* and *\\NTPROC* so it will only be described for *\\NTSPEC*.



13.6.1 Creating an NMR Superuser account

Before you install TOPSPIN, you have to make sure that there is an account for NMR Superuser. If there is none which you like to use, create a new one. According to your preference this can either be a local or a Domain account.

a) Creating a local NMR Superuser account

If you prefer a local NMR Superuser, do the following:

1. Log on at Windows XP Professional Workstation *\\NTSPEC* as the local Administrator or any other user who has User Administration rights, selecting *\\NTSPEC* as Domain.
2. Open the User Manager and create an account for the NMR Superuser, e.g. with the name *nmrsu*. (see also chapter and 9.1).

b) Creating a Domain NMR Superuser account

If you prefer a Domain NMR Superuser, do the following:

1. Log on at the Domain Controller *\\BOSS* as the Domain Administrator.
2. Open the User Manager and create an account for the NMR Superuser, e.g. with the name *nmrsu* (see also chapter and 9.1).

Note that the installation of TOPSPIN, which must be done as local Administrator, relies on the fact that the NMR Superuser was correctly installed. It cannot check if a Domain NMR Superuser really exists.

c) Installing TOPSPIN

The installation of TOPSPIN involves the following steps:

1. Log on as local Administrator on Windows XP Professional *\\NTSPEC*.
2. Install the TOPSPIN as described in chapter 6.4.

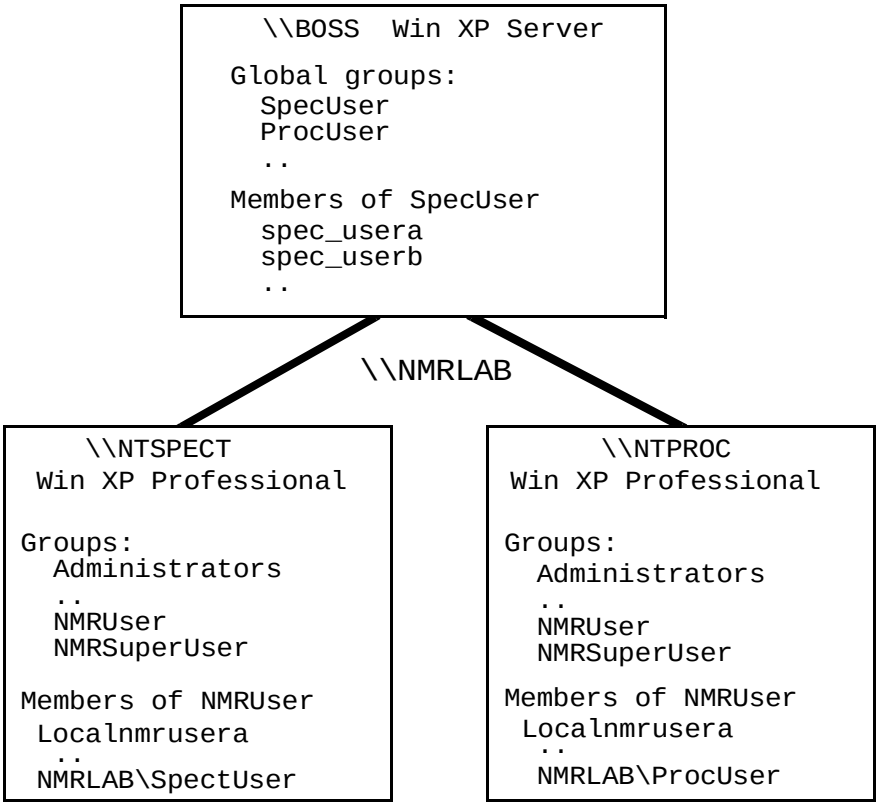
During the installation process, you will be asked for the NMR Superuser. Enter the name of the NMR Superuser account as created before (see chapter 13.6.1).

After the installation process, NMR users cannot start TOPSPIN yet. First they must be added to the local group NmrUser. Users with a local account, e.g. localnmrusera can simply be added to NmrUser as described in chapter 9.1.3. However, for users with a Domain account, which is typical in a Domain scenario, we recommend to use global groups as described in chapter 13.6.2.

13.6.2 Installing global user groups

The TOPSPIN installation program creates a local group NmrUser. Each user who wants to use TOPSPIN must be a member of this group. Domain users could be added individually to the local group NmrUser but, in a network with many Workstations and varying users, this would be an elaborate task. Therefore, we recommend to create so called global user groups. Global groups are created by the Domain Administrator on the Domain Controller. Each global group contains users who are allowed to do certain tasks, e.g. start TOPSPIN on a specific spectrometer or datastation. These global groups are then added to the local group

NmrUser on the various Workstations in the network. In our example, the Domain Administrator creates the global groups *SpecUser*s and *ProcUsers* which are then added to the local group NmrUser on *\\NTSPEC* and *\\NTPROC* respectively. After that, for example, the global user spec_usera can control the spectrometer from Workstation *\\NTSPEC*. By managing these global groups on the Domain Controller, the Domain Administrator can control which users can use the spectrometer and which can use the datastation. In practice, one global group will be added to the local group NmrUser on several Workstations and NmrUser on one Workstation can contain several global groups.



The installation of the global user groups involves the following steps:

1. Log on at the Domain Controller as Domain Administrator.

2. Create the global groups *SpecUser* and *ProcUser*.

3. Log on as local Administrator at workstation *NTSPEC*, selecting *NTSPEC* as Domain.
4. Add the global group *NMRLAB\SpecUser* to the local group *NmrUser* as described in chapter 9.2.4.
5. Repeat step 3 and 4 for *NTPROC* adding *NMRLAB\ProcUser* to the local group *NmrUser.*

13.6.3 Check for the HOME directory of every nmr users

There are two possibilities for the HOME directory of an user, local on every PC or fixed on one PC in the domain. Bruker supports both scenarios, the last one is a little bit more convenient, because the resource file (used by command 'setres') of TOPSPIN is stored in the home directory of the user. If there are individual settings it is easier to have to create this file only once and use it on all TOPSPIN installations of the windows domain.

Note that the configuration of TOPSPIN relies on the fact that the given HOME directory of an user exists. The HOME directory cannot be created by TOPSPIN.

Chapter 14

Installing a Printer

Printers must be installed at a Windows XP level and can then be used in TOPSPIN and TOPSPIN PLOT EDITOR.

14.1 Installing a new local printer

Installing a local printer implies installing the software, e.g. the printer driver for that printer. You can get printer drivers from various sources:

1. From a CDROM or floppy which was delivered with the printer:
   Please follow the instruction in the printer installation guide. If you do not have one, just insert the floppy or CDROM. The ***Setup*** program might start automatically. If it does not, open the Explorer and find a file named `Setup` or `Install` and click it.
2. From the Web:
   Just go to the manufacturers Web home page, e.g. `www.hp.com`, `www.canon.com` or `www.epson.com` and look for **Download** or **Drivers**. Usually, an executable file can be downloaded which can be unpacked and installed, simply by clicking on it.
3. From the Windows XP CDROM:
   If you do not have a CDROM or floppy with printer software and no Web access you can install a printer driver from your Windows XP CD. You will get

a list of printers for which a driver was available at the time your Windows XP version was released. If your printer type does not appear, you can select a related printer. However, Bruker BioSpin does not guarantee that this will work (see chapter 14.1.1 for installation instructions). Note:

Bruker BioSpin does not supply printer drivers for Windows XP!

14.1.1 Installing a printer from the Windows XP CDROM

A large number of printer drivers are available on the Windows XP CDROM. Note that these are the drivers which were available at the time Windows XP was released. For older printers these are usually valid. For newer printers the drivers might not be on the CD or better drivers might be available. Please use drivers delivered with the printer or from the Web whenever possible.

You can install a printer from the Windows XP CD as follows:

1. Log in as Administrator

2. Click **Start** → **Printers and Faxes**

3. A window '*Printers*' will appear:

- Double-click the icon **Add Printer**

4. A window '*Add Printer Wizard*' will appear: → Click **NEXT**

a) Click **Local Printer**, enable **Plug and Play** search mode if you want that the system looks for a new printer → Click **Next**

b) A window '*New Printer Detection*' will appear

- if the system finds a right printer → Click **Next**
- if the system does not find a printer define it manually during the next steps → Click **Next**

c) Select the port to which the printer is connected → **C**lick **Next**

d) In the field **Manufacturers**: select the manufacturer of the printer, e.g. HP

e) In the field **Printers**: select the type of the printer

If your printer does not appear in the list, select a related printer type or click **Cancel** and get the driver from the Web.

f) Click **Next**

g) In the field **Printer Name**: enter the name under which you want to use the printer (or accept the default name)

h) If other printers are already installed, you will be asked if the new printer must be the default printer:
   - If you want to use this printer as default printer → Click **Yes**
   - If you do not want to use this printer as default printer → Click **No**

i) Click **Next**

j) '*Printer Sharing*': Do one of the following:

   If the printer must be available for other computers in the network:
   - Click **Shared**
   - In the field **Share Name**: enter the name by which the printer can be accessed from a remote host, e.g. *viola_deskjet*
   - Click **Next**
   - A window '*Location and Comment*' appears. Write in some informations about the location, the printer administrator and individual printer specifications (e. g. the fax-default-printer etc.) → Click **Next.**

   If this printer should only be used on the local computer:
   - click **Not shared**.

k) Click **Yes** (to print a test page) → Click **Next** → Click **Finish**

5. If the window '*Insert disk*' appears:
- Insert the CDROM '*Windows XP Professional*' → Click **OK**

6. A window '*Files Needed*' will appear:
- Click **OK** (to copy the Driver files for your printer from the CD)

7. A new icon will appear in the window '*Printers*' (see step 3):

a) Click the right mouse button on the new printer's icon

b) Click **Printing Preferences** in the pop-up menu

8. A window '*Printing Preferences*' will appear:

a) Click **Advanced**

a) Click in the Field **Paper Size**

b) Select the correct paper size for your printer

c) Click **OK** → **OK**

Step 8 makes sure that applications like Word, Excel, Paint and TOPSPIN ... will use this paper size as default.

14.2 Remote printing from a PC to a PC

14.2.1 On the PC to which the printer is physically connected

If the printer is not installed yet:

- Install the printer as described in chapter 14.1. During this installation you have to choose between 'shared' and 'not shared'; click **Shared**

If the printer is already installed as a local printer:

a) Log in as Administrator

b) Click **Start** → **Printers and Faxes**

c) Click the right mouse button on the printer icon and select **Sharing ...**

d) A window '<*printer name*> *properties*' will appear:

- Click **Shared**
- In the field **Share Name**: enter the name under which the printer can be accessed on the network, e.g. *viola_deskjet*
- Click **OK**

e) Close the window '*Printers*' by clicking the **X** button

14.2.2 On the PC from which you want to print

1. Click **Start** → **Printers and Faxes**

2. A window '*Printers*' will appear:

- Double-click the icon **Add Printer**

3. A window '*Add Printer Wizard*' will appear:

a) Click **Network printer**

b) Click **Next**

c) A window '*Locate your printer*' will appear, enable one of the three fields under the point '*What Do You Want To Do*'

- '*Find a Printer in the Directory*' is a powerful search tool that is looking for a printer with the properties you want in the active directory if you are member of domain
  - Click **Next**, a window '*Find Printers*' will appear:

- Choose the domain path in the field '*In*'
- In the menu '*Features*' you have the possibility to enable some additional search modes like resolution, paper size etc.
- Click **Find Now**

- '*Type the Printer Name ...*'
  - Use this option if you already knows whats the name of the printer you want to install (use the form //<Print-Server>/<Printer-Name>) or if you want to start a search in the subdomain of your network
  - Click **Next**
- '*Connect to a Printer ...*'
  - Use this option if you want to connect to a internet printer that has an own URL address

! Wait until list of shared printers on that UNIX host appears. If this list does not appear within one minute, click the **Network Connections** icon on the desktop and try to connect to the remote host. Then go back to the window '*Connect to printer*', click the remote host again and see if get a list of shared printers now.

4. The window '*Add Printer Wizard*' will appear:

a) Do one of the following:
- Click **Yes** if you want to use this printer as default printer
- Click **No** if you do not want to use this printer as default printer

b) Click **Next**, click **Finish**

14.3 Remote printing from a UNIX host to a PC

14.3.1 On the PC to which the printer is physically connected

Install the printer as described in chapter 14.2.1.

1. Log in as Administrator

2. Insert the CDROM '*Windows XP Professional*'

3. Close the window '*Windows XP CDROM*' by clicking **Exit**

4. Click **Start** → **Control Panel** → **Network Connection**

5. A window '*Network and Dial-up Connection*' will appear:
   - Click on the pull down menu **Advanced** → **Optional Network Component**
6. A window '*Optional Network Component*' will appear:
   - Enable **Other Network File and Print Services**
   - Click on **Networking Services** to highlight it then click **Details**
     - enable **Simple TCP/IP Services** → **OK**
   - The check box for **Other Network File and Print Services** is now white and that one for **Networking Services** grey and both have a tick, click **Next**
7. Click **Start** → **Control Panel** → **Administrative Tools** → **Services**
8. A window '*Services*' will appear:

   a) Scroll down and check the following entries:
      - Simple TCP/IP Services
      - Print Spooler
      - TCP/IP Print Server

      If one of these entries is set to **manual**:
      - Click that entry to highlight it
      - Click **Action** → **Properties** → **Startup type** → select **Automatic** → **OK**
9. Click **Start** → **Turn Off Computer** → **Restart** → **Yes**

14.3.2 On the UNIX host from which you want to print

On the UNIX host, you must setup a network printer as follows:

1. Open a UNIX shell
2. Become superuser; type **`su`**
3. Edit the file `/etc/printcap` and make an entry like:

```
laserjet|HP :\
:rm=viola.netx.applic.com:\ [1]
:rp=hplj4ml:\
:sd=/usr/spool/lpd/hplj4ml:\
:sh:
```

1. Depending on your network you must enter hostname or hostname.domainname

where:

- *laserjet* is the name for the printer on the UNIX host
- *viola.netx.applic.com* is the hostname.domainname of the PC
- *hplj4ml* is the name of the printer on the PC

4. Create the spooling directory which is specified in `/etc/printcap`:

a) **`mkdir -p /usr/spool/lpd/hplj4ml`**

b) **`chown daemon.daemon /usr/spool/lpd/hplj4ml`**

c) **`chmod 770 /usr/spool/lpd/hplj4ml`**

More information on network printing under UNIX can be found in the manual `netprint` which is available on:

```
http://www.bruker-biospin.de/NMR/nmr-
    softw/passwd/docu/index.html
```

and as '*Network Printing*' in the TOPSPIN online help.

14.4 Remote printing from a PC to a UNIX host without Samba

Remote printing from a PC running Windows XP on a printer connected to a UNIX host can be realized in two different ways:

- by installing the Microsoft TCP/IP Printing package on the PC
- by installing Samba on the UNIX host (see chapter 14.5)

The first method is easier to install. The second method has advantages if you also want to use Samba's capability to share UNIX directories with Windows XP hosts.

14.4.1 Configuring the PC from which you want to print

1. Log in as Administrator

2. Insert the CDROM '*Windows XP Professional*'

3. Close the window '*Windows XP CDROM*' by clicking **Exit**

4. Click **Start** → **Control Panel** → **Administrative Tools** → **Services**

5. A window '*Services*' will appear:

Do you see an entry Microsoft TCP/IP Printing?

Yes? → Click **Cancel** and continue with step 6.

No? → Go to chapter 14.3.1

6. Click **Start → Printers and Faxes**
7. A window '*Printers*' will appear:
   - Double-click the icon **Add Printer**
8. A window '*Add Printer Wizard*' will appear:
   a) Click **Next → Local Printer**, disable '**Automatically detect and install my Plug and Play Printer**', click **Next**
   b) Enable **Create New Port** select Type **LPR Port → Next**
9. A window '*Add LPR compatible printer*' will appear:
   a) Enter the name of the LPD server (the UNIX host)
   b) Enter the name the printer has on the UNIX host[1]
   c) Click **OK**
   d) Close the window '*Printer Ports*' by clicking **Close**
10. In the window '*Add Printer Wizard*':
   a) Click **Next**
   b) In the field **Manufacturers**: select the manufacturer of your printer
   c) In the field **Printers**: select your printer type
   d) Click **Next** (to accept the default printer name)
   e) Click **Not shared → Next → Finish**
   f) Answer the question '*Was the test page printed correctly?*' with **Yes**
   g) Close the windows '*Printers*' and '*Control Panel*' by clicking the **X** button

14.4.2 Configuring the UNIX host to which the printer is physically connected

1. Open a UNIX shell
2. Become superuser; type **`su`**
3. Edit the file `/etc/printcap` and make an entry like:

```
laserjet|HP :\
 :lp=/dev/plp:\
 :sd=/usr/spool/lpd/laserjet:\
 :sh:\
```

1. You can check this name by logging in on the UNIX host and entering 'lpstat -t'

```
:sf:
```

where:

- `laserjet` is the name for the printer on the UNIX host
- `lp` is the port where the printer is physically connected

4. Create the spooling directory which is specified in `/etc/printcap`, e.g.:
   a) **`mkdir -p /usr/spool/lpd/laserjet`**
   b) **`chown daemon.daemon /usr/spool/lpd/laserjet`**
   c) **`chmod 770 /usr/spool/lpd/laserjet`**
5. Edit the file `/etc/hosts.lpd` and enter two lines like:

```
viola
viola.netx.applic.com
```

where *viola* is the hostname and *netx.applic.com* the domainname of the remote PC.

14.5 Remote printing from a PC to a UNIX host with Samba

This chapter describes how you can install a printer on a Windows XP computer, when the printer is physically connected to a UNIX host, e.g. an SGI. The method described here involves the installation of Samba, which also allows you to access directories on the UNIX host from the Windows XP host. Alternatively, you can install the printer without using Samba, as described in chapter 14.4.

14.5.1 Configuring the UNIX host to which the printer is physically connected

1. Get the Samba package from the Internet and install it as described in chapter 13.4.3.
2. In the SWAT (see chapter 13.4.3) choose the printer according to your preference. All Printer that are defined in the printcap occurs in the pop-up menu.
3. Reboot the UNIX workstation

14.5.2 Configuring the PC from which you want to print

1. Click **Start** → **Printers and Faxes**
2. A window '*Printers*' will appear:
   - Double-click the icon **Add Printer**

3. A window *'Add Printer Wizard'* will appear:

a) Click **Network printer**

b) Click **Next**

c) A window *'Locate your printer'* will appear, enable one of the three fields under the point *'What Do You Want To Do'*

- *'Find a Printer in the Directory'* is a powerful search tool that is looking for a printer with the properties you want in the active directory if you are member of domain
  - Click **Next**, a window *'Find Printers'* will appear:
    - choose the domain path in the field *'In'*
    - In the menu *'Features'* you have the possibility to enable some additional search modes like resolution, paper size etc.
    - Click **Find Now**
- *'Type the Printer Name ....'*
  - use this option if you already know the name of the printer you want to install (use the form //<Print-Server>/<Printer-Name>) or if you want to start a search in the subdomain of your network
  - Click **Next**
- *'Connect to a Printer ...'*
  - Use this option if you want to connect yourself to a internet printer that has an own URL adress

Wait until list of shared printers on that UNIX host appears. If this list does not appear within one minute, click the **My Network Place** icon on the desktop and try to connect to the remote UNIX host. Then go back to the window *'Connect to printer'*, click the remote UNIX host again and see if get a list of shared printers now.

- Double-click the printer connected to the UNIX host, e.g. **laserjet**

4. A message about a missing NULL printer driver will appear:

- Click **OK**

5. A window *'Add Printer Wizard'* will appear:

a) In the field **Manufacturers**: select the manufacturer of the printer, e.g. **HP**

b) In the field **Printers**: select the type of the printer

If your printer does not appear in the list, select a related printer type or click **Cancel** and get the driver from CDROM or from the Web.

c) Click **Next**

d) If other printers are already installed, you will be asked if the new printer must be the default printer:

- If you want to use this printer as default printer: click **Yes**
- If you do not want to use this printer as default printer: click **No**

e) Click **Next**, click **Finish**

14.6 Installing a printer with a JetDirect print server

If your printer is connected to the network via a HP JetDirect print server, you must install it in the following way:

1. Log in as Administrator

2. Install the Service Microsoft TCP/IP Printing as described in chapter 14.3.1.

3. Click **Start → Printers and Faxes**

4. A window '*Printers*' will appear:

- Double-click the icon **Add Printer**

5. A window '*Add Printer Wizard*' will appear:

a) Click **Next → Local Printer**, disable '**Automatically detect and install my Plug and Play Printer**', click **Next**

a) Enable **Create New Port** select Type **LPR Port → Next**

6. A window '*Add LPR compatible printer'* will appear:

a) In the field **Name or Address of server providing lpd**: enter the name or IP address of the Print Server.

b) In the field **Name of printer or print queue on that server** you must enter:

- **raw1** if you have an internal JetDirect adapter
- **raw1**, **raw2** or **raw3** if you have an external JetDirect print server, depending on the JetDirect port to which the printer is connected.

c) Click **OK**

7. In the window '*Printer Ports*':
   - Click **Close**
8. In the window '*Add Printer Wizard*':
   - Click **Next**
9. Continue the installation as described in chapter 14.1.1, step 4d.

Part III

Tips, Tricks and Troubleshooting

Chapter 15

Troubleshooting

15.1 General checks

15.1.1 Windows XP Services

The TOPSPIN requires the following Windows XP Services to control a spectrometer. Proceed as follows:

1. Click **Start** → **Control Panel** → **Administrative Tools**
2. Double-click **Services**
3. A window '*Services*' will appear:

   At least the following services should appear with status **Started**:

   - Bfs
   - Bootparam
   - Bruker FLEXlm License Server (only if the PC has a local license. If the license server is a remote machine, the FLEXlm service has to be started only there)
   - Hummingbird Inetd
   - Hummingbird NFS Server

- Hummingbird Port Mapper
- NuTCRACKER Service
- Schedule

Note that this list only contains the Services required for the TOPSPIN. Several other Services are required for Windows XP and possibly for other software packages on your system.

4. If one or more of these services are not running:
   - Reboot the computer and check again
5. If rebooting does not solve the problem, then proceed as follows:

   If the NuTCRACKER Service, bfs and/or bootparam are not running:
   - Re-install TOPSPIN and DISKLESS (see chapter 6.4)

   If the Hummingbird NFS Server and/or Port Mapper are not running:
   - Remove the NFS Server directory

     (normally `C:\Program Files\NfsSrvr.nt`)
   - Re-install the NFS Server (see chapter 4.3)
6. Carefully check the NFS Server configuration (see chapter 6.6).

15.1.2 The Event Viewer

If you have any problems on your Windows XP host, it is always a good idea to look at possible Events which caused them:

1. Click **Start** → **Control Panel** → **Administrative Tools** → **Event Viewer**
2. A window *'Event Viewer'* will appear:
   - Click **Application Log** to see Application Events
   - Click **System Log** to see System Events
   - Click **Security Log** to see Security Events
3. Double-click on an Event to get more information on it.
4. Note that Events do not necessarily indicate problems. If fact, there are three type of events: *Information*, *Warning* and *Error.*

To prevent the Event Log from getting full we recommend to do the following:

5. Click on one of the three Log's, e. g. **System Log** → **Action** → **Properties**

6. A window '*System Log Properties*' will appear:
7. Set the '*When maximum log size is reached*' to one of the following:
   - **Overwrite Events as Needed**
   - **Overwrite Events Older than 7 Days**

15.2 TOPSPIN does not start

If TOPSPIN does not start, you should first look for an error message in the window where the TOPSPIN startup messages appear. Then check if you have one of the following problems:

1. A window '*`Choose Server or File`*' appears:

   The file `license.dat` was not found. You might have one of the following problems:

   - The Flexlm license manager is not installed

     → Install Flexlm license manager from the TOPSPIN CDROM
   - `license.dat` has been deleted or renamed

     → Setup the file `license.dat` as described in chapter 7.2.3.
   - `license.dat` has a (hidden) extension `.txt` or `.example`

     → Rename the file to `license.dat`

2. '*`NuTCRACKER fatal error; failed to register this Service`*'

   Click **OK**, then just try starting TOPSPIN again, it might work the second or third time. This error appears if TOPSPIN started immediately after booting the PC and so the Nutcracker Service is not yet running. If this does not work:

   a) Click **Start** → **Control Panel** → **Administrative Tools**

   b) Double-click **Services**

   c) A window '*Services*' will appear: → Select **Nutcracker**, click **Start**

If the service Nutcracker does not start, there might be 2 different causes:

a) Certain system software was installed after installing an Windows XP Service Pack → Re-install the Service Pack

b) TOPSPIN was removed and re-installed without rebooting the computer in between. → Remove TOPSPIN, reboot and re-install TOPSPIN

3. *`NUTCRACKER OE will not install with an error message that the services 'workstation' and 'server' are not running.`*

Service 'workstation' is still active but the service 'server' does not appear in the list of services. Please check the network configuration, if the option **File and Printer Sharing for Microsoft Networks** is disabled or de-installed. The consequence is that the service 'server' is not available.

4. If hostid '*0*' or '*ffffffff*' occurs:

You may run Windows XP and your network-adapter has no link to the network. Establish an link to the network or install the

`NWlink IPX/SPX/NetBIOS Compatible Transport Protocol:`

a) Click **Start** → **Control Panel** → **Network Connections**

b) Right-click **Local Area Connection xxx**

c) Click **Properties** → **Install...** → **Protocol** → **Add**

d) The *`Select Network Protocol`*-menu will appear after some seconds. Click **NWlink ...** → **OK**

e) After some seconds the Properties-menu will reappear → Click **Close**

5. *`'Cannot connect to license server... WinSock Error code...'`*

The file `license.dat` was found, but Flexlm does not run. Maybe:

a) Flexlm is not installed: → Install Flexlm from the TOPSPIN CDROM

b) the Service (Bruker) Flexlm license server is not running:

→ Click **Start** → **Control Panel** → **Administrative Tools**

- Double-click **Services**
- A window '*Services*' will appear:
- Select **Flexlm**..., click **Start**

6. *`'Server node is down or not responding (-96,379)'`*

The server could not answer because he is down, the entry <SERVER-NAME>

in '`license.dat`' is wrong or the server has been wrong configured:

→ Check if the server in the '`license.dat`' file is down:

- Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
- type '**`ping <SERVER-NAME>`**' and check if the correct reply occurs:

a) A reply like this:
`Reply from <SERVER_IP_ADRESS>: bytes=32 time<10ms TTL=128` shows that the server is okay.

b) A reply like this: *'`Request timed out`'* shows that the server is down

c) A reply like this: *'`Bad IP address <SERVER-NAME>`'* shows that the <SERVER-NAME> is wrong or the server is not correctly configured.

→ Check if the entry of the server in the '`license.dat`' file is wrong (wrong name, blanks, ...), if so correct it.

→ Check if the server has a wrong configuration, e. g. TCP/IP protocol or NetBIOS network service is not installed. For this you should have a look at:

- **Start** → **Control Panel** → **Network Connections**
- Click on the LAN entry of your ethernet card → **File** → **Settings**
- A window '*Local Area Connections Properties*' will appear
- Look if there is an entry '*Internet Protocol (TCP/IP)*'
  - Yes? click on it to highlight the entry → **Properties**
  - No? see 13.1.1
- A window '*Internet Protocol (TCP/IP) Properties*' will appear
- Click on **Advanced**
- A window '*Advanced TCP/IP Settings*' will appear
- make sure that the entry '*Enable NetBIOS over TCP/IP*' is enabled

Also click:

- **Start** → **Control Panel** → **Administrative Tools**
- Double-click **Services**

- A window *'Services'* will appear:
  make sure that **server** and **TCP/IP NetBIOS** have the status *'started'*

7. *'`Failed to register Kernel Service`'*

the Service Nutcracker Kernel is probably not running:

→ Click **Services** in the **Control Panel** → Select **Nutcracker** → Click **Start**

8. *'`Cannot find resolution file`'*

→ Reboot the computer and try again

9. *'`Invalid license key (inconsistent license key)`'*

The file `license.dat` might contain one of the following errors:

- The hostid in the SERVER line is wrong
- The FEATURE line contains the wrong license key, the wrong date and/or the wrong number of licenses
- The hostid is appended at the end of the FEATURE line
  (this is correct for *Node Locked* licenses but not for *Floating* licenses, see chapter 7.1)

10. *'`Invalid data returned from license server`'*

- Hostname in the file `license.dat` is incorrect

11. *'`Invalid host`'*

- The file `license.dat` contains additional characters at the end of the FEATURE line (after "")

For more information on the Flexlm license manager:

Click **Start** → **run** enter **`c:\flexlm\bruker\help\index.htm`** → Click **OK**

15.3 TOPSPIN troubleshooting

TOPSPIN should not get into any trouble in general!

Nevertheless, if your current TOPSPIN session has a problem, you can find in this chapter some instructions how to get rid of this situation.

In order to stop TOPSPIN in case of any problems, the first thing to know is, that

TOPSPIN is working with a client / server structure. The server is the program itself and the client is the graphical interface. It is possible to exit each of them separately. It is also possible to start more than one client (graphical interface). This feature is used for the remote control but can also be very useful for troubleshooting (see below)!

- The client (= graphical user interface of TOPSPIN*)* can be stopped without touching a running acquisition.
- Stopping the program itself will also stop a running acquisition.

15.3.1 Troubleshooting while no acquisition is running

The most convenient way to get rid of a problem inside TOPSPIN is, to stop the complete program. For this you can do the following steps. These steps are increasingly drastic.

1. Press the **Esc** key.

This will not kill TOPSPIN and might enable input again.

2. Enter ***exit*** in the TOPSPIN command line or press the ***X*** in the upper right corner of the program window.

Is the TOPSPIN window closed?

- Yes? Start TOPSPIN once again, in case there will be still some problems go ahead with step 3.
- No? Go ahead with step 3.

3. Stop the current TOPSPIN window and start a new one

a) Enter in the TOPSPIN command line:

```
logoff
```

b) Open a **Command Prompt** (Click **Start** → **All Programs** → **Bruker TOPSPIN** → **Bruker TOPSPIN x.y** → **Bruker Utilities** → **Command Prompt**) and start a second TOPSPIN:

```
topspin -client
```

Has the first TOPSPIN window been closed and does the second one work fine?

- Yes? The problem is solved you can go ahead with TOPSPIN.
- No? Go ahead with step 4.

4. Stop all TopSpin windows and end the program itself

a) Try to stop all TOPSPIN windows by enter the command:

logoff

in the TOPSPIN command line.

b) Kill TOPSPIN in the following way:

a) Press **CTRL+SHIFT+ESC** to start the Task Manager

b) Click **Applications**

c) Click **Bruker TOPSPIN 1.x**

d) Click **End Task**

e) Go to the Bruker Utilities:

- Click **Start** → **All Programs** → **Bruker TOPSPIN** → **Bruker TOPSPIN x.y** → **Bruker Utilities**
- A window *'Bruker Utilities'* appears.
- Double click ***Miscellaneous***
- Double click the entry:

shmrm

15.3.2 Troubleshooting while an acquisition is running

The difference to the situation that no acquisition is running is, that you can try to stop only the graphical user interface without stopping the acquisition. Step 1 does not stop the acquisition, step 2 will stop also the acquisition.

1. Stop the current TOPSPIN window and start a new one

a) Enter in the TOPSPIN command line:

logoff

b) Open **Command Prompt** (Click **Start** → **All Programs** → **Bruker TOPSPIN** → **Bruker TOPSPIN x.y** → **Bruker Utilities** → **Command Prompt**) and start a second TOPSPIN:

```
topspin -client
```

Has the first TOPSPIN window been closed and does the second one work fine?

- Yes? The problem is solved you can go ahead with TOPSPIN.
- No? Go ahead with step 2.

2. Stop all TOPSPIN windows and end the program itself

a) Try to stop all TOPSPIN windows by enter the command:

logoff

in the TOPSPIN command line.

b) Kill TOPSPIN in the following way:

a) Press **CTRL+SHIFT+ESC** to start the Task Manager

b) Click **Applications**

c) Click **Bruker TOPSPIN 1.x**

d) Click **End Task**

e) Go to the Bruker Utilities:

- Click **Start** → **All Programs** → **Bruker TOPSPIN** → **Bruker TOPSPIN x.y** → **Bruker Utilities**
- A window '*Bruker Utilities*' appears.
- Double click ***Miscellaneous***
- Double click the entry:

shmrm

15.4 Send debug information to Bruker BioSpin

If you are in a situation, that TOPSPIN problems appear periodically you can send the information about this situation to Bruker BioSpin. To get the information go into the error message in the window where the TOPSPIN startup messages appear. and press the keys '**Ctrl**' and '**Break**' simultaneously. This will create a debug output inside the shell. Please copy this output into an email and send it to this address:

`nmr-software-support@bruker-biospin.de`

For a complete debugging it is useful to attach the history file of the TOPSPIN session. For this attach the following two files:

`<TOPSPINHOME>/prog/curdir/<USER_NAME>/history`

`<USER_HOME>/.topspin-<PC_NAME>/prop/protocol.txt`

15.5 Communication problems between PC and CCU

If the acquisition (**zg**, **gs**, **wobb**) and/or the configuration (**cf**) fails, you might have a communication problem between the PC and the spectrometer CCU.

15.5.1 Hardware related problems

1. Check if the Ethernet cable between the PC and the CCU is properly connected.

→ Remove and re-connect the Ethernet cable.

2. Does the connection light come on if you connect CCU and ethernet board in the PC?

a) If the light is off

The connection light is one of the three LEDs that most Ethernet cards have. One of them, usually in yellow, lights up the same moment that both ends of the respective cable are connected to life devices like a hub or wall socket or a computer.

- Check the cable or the Ethernet card; with some cards you need to reboot the PC with CCU and Ethernet-board being connected to make the initial connection. If the PC is started without any cable connected to the board some configurations will disable the card unless configuration takes place (makes sense for unused cards, however forces us to re-boot more often than we might want to).
- In some cases the auto-negotiate protocol of certain cards doesn't work. That means CCU can't find out whether to go for 10baseT or 100baseT. Some of the newer Ethernet cards allow you to switch the auto-negotiate off. Software configuration allows you to set a fixed speed of 10. In some cases you can also force a card into 10Mbps by putting a hub (a 10Mbps hub!) between PC and CCU. The hub will tell the card to switch to 10Mbps and CCU gets around auto-negotiate, too.

If the light still doesn't come on, please connect the Ethernet board with some operational network (e.g. corporate network). If you get a physical connection (light goes on) obtain a temporary IP address for the PC and install the card, network, netmask, DNS etc to the point where you see the rest of the company through the 'network neighborhood' of your PC. This will make sure that your card works at all. Then switch back to the IP/netmask for spect and reboot PC. Is the light on? If not, get a new Ethernet card.

b) If the light is on:

At this point you know that the physical connection is intact (that is: the connection light on the PC's Ethernet board came on). There are two possibilities to check from here:

- CCU is indeed booting OK, yet you can't access it for some reason.
- CCU really does not boot and you have to find out why.

Before you proceed you might want to quickly check the settings in NFS Maestro. Call it from the Control Panel (HCL NFS Server) and you need to see the configuration given in chapter 6.6. If settings have to be altered, do this, reboot the PC and then the CCU before checking again.

- The minimum test is this: Try to ***ping spect*** and then to ***telnet spect*** (see chapter 8.3). Here is how to proceed:

If you can `ping` and `telnet` and get spect's login prompt you should be able to run TOPSPIN from here. You are all set.

If you can `ping` but cannot `Telnet` to CCU the physical connection is all right but CCU doesn't boot. Please connect a monitor cable to CCU and open a Hyper Terminal connection. HyperTerminal is Windows's text terminal emulator and it comes with every copy of Windows. The details are in chapter 15.5.5

If you can't even `ping` CCU try a new Ethernet cable and if it still doesn't work try another type of Ethernet card.

15.5.2 Software related problems

Please check if the required Services are running as described in chapter 15.1.1.

15.5.3 View the output of the CCU console

In order to view the output of the spectrometer CCU, you must connect the COM2 port of the PC to tty00 of the CCU. The hyper terminal application can be used to make the output of the CCU visible on the PC (this has the same function as **`cu`** and **`kermit`** on UNIX systems).

15.5.4 Configuration of HyperTerminal

1. Click **Start** → **All Programs** → **Accessories** → **Communications** → **HyperTerminal**
2. If you do this for the first time HyperTerminal will ask for some informations in

the window '*Location Information*'.Type in your ZIP-code and click **OK**

3. A window '*Phone And Modem Options*' will appear → **OK**

   Then establish a new connection:

4. A window '*Connection Description*' will appear:
   a) In the Field **Icon**: click any icon you decide for
   b) In the field **Name**: enter **CCU**
   c) Click **OK**
5. A window '*Connect to*' will appear:
   a) Click in the field **Connect using**: select **COM2**
   b) Click **OK**
6. A window '*COM2 Properties*' will appear:
   a) Click in the field **Bits per second** and select **9600**
   b) Click in the field **Flow Control** and select **Xon/Xoff**

      (the other settings remain unchanged: Data bits 8, Parity None, Stop bits 1)
   c) Click **OK**

      → the output of the CCU will appear in the window '*CCU Hyper Terminal*'
7. Click **File** → **Save**
8. Click **File** → **Exit**
9. Answer the question '*Are your sure you want to disconnect now?*' with **Yes**

15.5.5 Usage of Hyper Terminal

1. Click **Start** → **All Programs** → **Accessories** → **Hyperterminal** → **CCU.ht**
2. A window CCU Hyper terminal will appear in which you see the output of the CCU.

   If the CCU is booted, you will see a login prompt and you can log in as root. If the CCU is not booted you can push the reset button on the CCU and view the boot process. The boot process is shown below. The messages '*Fast ethernet...*' only occur for CCU/9 and indicate whether you have a 10 MBit/s or 100 MBit/s ethernet connection. Note that a UNIX pathname for the DISKLESS program is shown. Do not worry about this, it is automatically interpreted as an Windows XP path like: C:\Bruker\Diskless...

   ```
   Autoboot: Waiting to load bfs()/usr/diskless/cli-
   ```

```
ents/spect/root/unix.r4600_std (
CTRL-C to abort)
loading


Fast ethernet (FEN): 100 MBit/s, half duplex
   ---1---
Obtaining  /usr/diskless/clients/spect/root/unix.r4600_std
from server 'hostname'
833328+107984+827152 entry: 0x80021000
CPU: MIPS .... Processor Chip Revision: ...
FPU: MIPS .... Floating Point Unit [CP1] Revision: ...

RISC/os Release 4_52 mips Version UMIPS
Total real memory = 16777216
Available memory  = 14360576
Root on nfs file :,Swap on nfs f
Fast ethernet (FEN) : 100 MBit/s, half duplex
   ---2---
hostname: spect
domainname: software.bruker.de
   ---3---
Root fstype nfs
Available memory  = 12713984

   ---4---
The system is coming up. Please wait.
/etc/init.d/sym_install start
/etc/init.d/sym_install calls sym_install
Adding swap device /swapfile
Fast ethernet (FEN) : 100 MBit/s, half duplex
Internet daemons: portmap inetd.
NFS daemons: nfsd biod lockd statd.
/tmp: Permission denied
/var/tmp: Permission denied
The system is ready:


spect Console login:
```

Booting might hang, stop (and print an error message) or go into an endless loop at one of the positions 1 through 3. This might be caused by one of the problems mentioned below. Check the indicated files and correct them if necessary or per-

form the indicated steps.

a) If booting stops at position ---1--- and you get the messages:

```
Fast ethernet (FEN): 100 MBit/s, half duplex
No server for /usr/diskless/clients/spect/root/un-
ix.r4600_std
BRUKER CCU R4600 Monitor
Version 5.40 MIPS OPT Wed Jun 11 19:30:43 MSZ 1997 root
Memory size: 16777216 (0x1000000) bytes, 16 MB
Icache size: .... (....) bytes
Dcache size: ..... (....) bytes
>>
```

then you might have one of the following problems:

- The Service *bfs* not running:

  Click **Start** → **Control Panel** → **Administrative Tools** → **Services** → **bfs** → **Start**

- The Diskless package is not installed (see chapter 6.4)
- The ethernet cable between PC and CCU allows no data throughput:

  - check the connection between the cable and the PC/CCU

  - check if the correct ethernet card is connected

  - check the configuration of the ethernet port (see chapter 13.1)

b) If booting stops at ---2--- you may have one of the following problems:

- The Service *bootparam* is not running:

  Click **Start** → **Control Panel** → **Administrative Tools** → **Services** → **bootparam** → **Start**

- The file `C:\Windows\system32\drivers\etc\Hosts` is wrong:

  It should contain the following entries:

  ```
  149.236.99.1 ASP_ST2
  149.236.99.99 spect
  ```

  Be sure that '`spect`' is the first entry after the number in this line

c) If booting stops at ---3--- you might have the following problem:

- The file `c:\Bruker\Diskless\WinApp\bootparams` is wrong. For a default installation it must contain the lines:

```
#
spect  root=ASP_ST2:C:/Bruker/Diskless/clients/spect/root \
       swap=ASP_ST2:C:/Bruker/Diskless/clients/spect/swap \
      dump=ASP_ST2:C:/Bruker/Diskless/clients/spect/dum
```

For a custom installation the path of Diskless can be different!

d) If booting hangs at ---3--- in a loop and you get the messages:

a) like this:

```
domainname: software.bruker.de
mount  root  ASP_ST2:C:/Bruker/Diskless/clients/spect
/root failed, rpc status 15
PANIC: vfs_mountroot: cannot mount root
syncing disks... done
```

then you might have one of the following problems:

- The Service Hummingbird NFS Server is not running

  Click **Start** → **Control Panel** → **Administrative Tools** → **Services** → **Hum. NFS Server** → **Start**

- The path `C:\Bruker\Diskless\clients\spect` is not exported

(see chapter 6.6).

b) like this:

```
domainname: software.bruker.de
mount  root  ASP_ST2:c:/Bruker/Diskless/clients/spect
/root failed, rpc status 2
PANIC: vfs_mountroot: cannot mount root
syncing disks... done
```

then you might have the problem that the drive letter of the diskless installation is written in lower case (maybe caused by a custom installation). To solve the problem you can either

- De-install Diskless and use for the new installation '*typical*' or make sure that the drive letter is upper case

or

- Open the file

  `c:\Bruker\Diskless\WinApp\bootparams`

  and change all drive letters to upper case

c) If booting stops at ---4--- and you get messages like this:

```
<date> INIT: Can't open /etc/ioctl.syscon. errno: 13
touch: /etc/mtab cannot create
mount: /etc/mtab: No such file or directory
<date> INIT: warning: /etc/ioctl.syscon does not exist, default settings assumed
<date> INIT: Can't open /etc/ioctl.syscon. errno: 13
<date> INIT: Cannot create /etc/utmp
<date> INIT: failed write of utmp entry: "   "
```

Please check diskless tree permissions and NFS User- and Group-Mappings (see Chapter 6.6)

d) If you see the message:

mount dumpfile ASP_ST2:C:/Bruker/Diskless/clients/spect/dump failed

during the boot process, you can ignore this. The CCU will boot anyway.

3. Click **File** → **Exit** to finish your Hyper Terminal session.

15.6 Troubleshooting for NMR-GUIDE

If you have some trouble with your installation of the NMR-GUIDE, please check the following :

1. Check for the NMR-GUIDE license (see chapter 7)

Edit the file C:\flexlm\Bruker\licenses\license.dat and check weather there is a FEATURE NMRGUIDE line. If not, enter the FEATURE line or apply for a license at

license@bruker.de

2. Check for all necessary components

- Internet Explorer $\geq$ 6.0 (see chapter 3)

3. Install the NMR-GUIDE program from the TOPSPIN CD once again and reboot. (This is necessary, because installation of the operating system components might have overwritten certain registry keys that are set during the NMR-GUIDE installation.)

4. Now try the NMR-GUIDE again

15.7 Bruker Service tools

Several tools for checking the spectrometer hardware are delivered with TOPSPIN. This includes tools for BSMS, HPPR, ACB, GRAD, HPCU, RX22. You can start a service tool as follows, for a full description see chapter 8.5:

1. Double-click the icon **Bruker Utilities** on the desktop
2. A window will appear with the icons Service tools, Test Tools etc.:
   a) Double-click **Service Tools** to get a list of service tools
   b) Double-click **Test tools** to get a list of test tools
3. A windows with the available tools will appear:
   - Double-click any icon to start the corresponding tool

15.8 Windows XP Service Pack

All PC's delivered by Bruker BioSpin have the latest Service Pack installed. It can also be downloaded from the Microsoft Web pages `www.microsoft.com` or `www.microsoft.de`.

For installation just follow the given instruction on the screen.

Under Windows XP it is not necessary to reinstall the service pack after e. g. configuring the network.

During the installation, you might get the message that files were detected which are not the original Windows XP files and which are also part of the Service Pack. Sometimes, these files are even newer than the ones in the Service Pack. This typically happens when you installed recent driver software. You are asked if these files should be overwritten. Bruker BioSpin recommends to answer this question with **No**, unless you are sure you want to update this file from the Service Pack.

15.9 Disk full or fragmented

If you have disk space problems, have a look at the Windows XP Online help:

Click **Start** → **Help** → **Index**

enter **`increasing disk space`** choose one subentry and click **Display**. If you want to defragment your disk see chapter 19.3. Note that NTFS partitions, which are required for TOPSPIN, suffer much less from fragmentation than FAT partition.

Furthermore, you might have to remove TOPSPIN data, e.g.:

1. Delete imaginary data using the ***`deli`*** command

   They are no longer needed for spectra which have been phase corrected.

2. Delete processed data using the ***`delp`*** command

   They can always be retrieved by reprocessing the data.

3. Delete raw data with the ***`del`*** command

   Please make sure you have a backup of the data.

15.10 Creating an Windows XP Boot Disk

You can use a Windows XP bootable disk to start the operating system on a computer running Windows XP. Use the procedures in this article to work around the following boot issues:

- Damaged boot sector.
- Damaged master boot record (MBR).
- Virus infections.
- Missing or damaged `ntldr` or `ntdetect.com` files.
- Incorrect `ntbootdd.sys` driver.

You cannot use the Windows XP boot disk to help resolve the following issues:

- Incorrect or damaged device drivers that are installed in the System folder.
- Boot issues that occur after you see the Windows XP startup (Osloader) screen.

15.10.1 PC is not booting from floppy?

In case it is not possible to boot the PC from a bootable floppy, this possibility might be disabled in BIOS. The following description shows how to enable the boot-from-floppy feature on a hp workstation xw4100 PC. On other PC's the procedure might be slightly different.

1. During boot time cancel the boot process and go into BIOS

   On different PCs there are different ways to do this, for example, on some PCs the boot sequence is interrupted with the **Delete** key rather than with the **F2** key.

2. Go to section

   Security → Boot Devices Security

3. Set *Floppy* to **Enabled**

Note: It is recommended to disable the boot-from-floppy feature after the boot process is done!

If it is enable, it is possible to get very easily a boot virus into BIOS, that can make your PC defective!

Another small advantage is, that if the BIOS feature above is enabled and a 'normal' floppy is inside the drive, booting the PC will stop and showing the information that a non bootable floppy is inside. If it is disabled booting the operating system will work with or without floppy.

15.10.2 Floppy boots Operating System from hard disk

You can create an Windows XP Boot Disk by formatting a floppy from within Windows XP and copying the following files from the root of an Windows XP boot partition (e.g. C:) to the floppy (Special note: the boot partition is the first partition which is read by bios. This is normally but not necessary the partition *'c:'*. If you installed Windows XP on a different partition e.g. *'d:'*, the following files are anyhow on *'c:'*.

- `ntldr`
- `ntdetect.com`
- `boot.ini`

If you are using SCSI disks with the SCSI BIOS disabled then also copy the file:

- `ntbootdd.sys`

a) Create a Boot Floppy Disk with the command prompt

Copy these files with command prompt is easier to describe than with the Windows explorer, because these are critical system files that are normally not shown in the explorer window.

1. Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
2. Type **`c:`**
3. Type **`dir /ah`** → you should see the necessary files
4. Type **`xcopy /h boot.ini a:`**
5. Type **`xcopy /h ntldr a:`**
6. Type **`xcopy /h ntdetect.com a:`**
7. If necessary (see above) type **`xcopy /h ntbootdd.sys a:`**

Now you can boot your PC from the Boot floppy. Be aware that this will only work if Windows XP is still on the hard disk. If Windows XP is not available or corrupt it must be repaired again from CDROM or from floppy.

b) Create a Boot Floppy Disk with the Windows Explorer

1. Format a floppy disk by using the Windows XP format utility.
2. Copy the `ntldr` and the `ntdetect.com` files from the I386 folder on the Windows XP Setup CD-ROM, Windows XP Setup floppy disk, or from a computer that is running the same version of Windows XP as the computer that you want to access with the boot floppy.
3. Copy the `boot.ini` file from a computer that is running Windows XP. Or create a `boot.ini` file, and then modify it to match the computer that you are trying to access. The following example works for a single-partition IDE drive with Windows XP installed in the \Windows folder, but the exact value in the [operating systems] section depends on the configuration of the Windows XP computer that you are trying to access:

```
[boot loader]
timeout=30
Default= multi(0)disk(0)rdisk(0)partition(1)\windows

[operating systems]
multi(0)disk(0)rdisk(0)partition(1)\windows="Windows XP"
```

If your computer boots from a SCSI hard drive, you may need to replace the multi(0) entry with scsi(0). If you are using scsi(x) in the `boot.ini` file, copy the correct device driver for the SCSI controller in use on the computer to the root of the Setup disk, and then rename it `ntbootdd.sys`. Change the disk(0) number to represent the SCSI-ID of the hard drive you want to

boot to. If you are using multi(x) in the `boot.ini` file, you do not need to do this.

4. Start your computer by using the floppy disk, and then log on to Windows XP.

15.11 Backup of Windows XP and TOPSPIN

The standard backup programs under Windows XP is called **`ntbackup`** which can be started by clicking:

Start → All Programs → Accessories → System Tools → Backup

Under Windows XP ntbackup is possible to use ZIP, tape and external hard disks as backup media.

You cannot choose a CD-R, CD-RW, or DVD-R device because ntbackup.exe does not support backing up to these devices. The **R**emovable **S**torage **M**anagement (RSM) does not have the ability to recognize these three devices as backup pool media. RSM regards CD-R, CD-RW, or DVD-R as just a file system-capable media type, but the Windows file system does not support formatting these media types. When it attempts to write an RSM free label, RSM does not succeed because the disc appears to be write protected. This means that RSM treats CD-R, CD-RW, or DVD-R media as a read-only media type even if you add them to the ntbackup media pool. Before you buy a tape drive, make sure it is compatible with your PC's interface(s); IDE and/or SCSI.

Bruker BioSpin recommends to make a regular backup of the partition(s) on which Windows XP and the TOPSPIN are installed.

15.11.1 Complete Backup of the PC

1. Click **Start → All Programs → Accessories → System Tools → Backup**
   → a window *backup* will appear
2. Click **Welcome → Backup Wizard**
   → a window *Backup Wizard* will appear → **Next**
3. Enable *Backup everything on my computer* → **Next**
4. Choose the media drive you want to store the backup → **Next**
5. Click '*Finish*' to start the backup

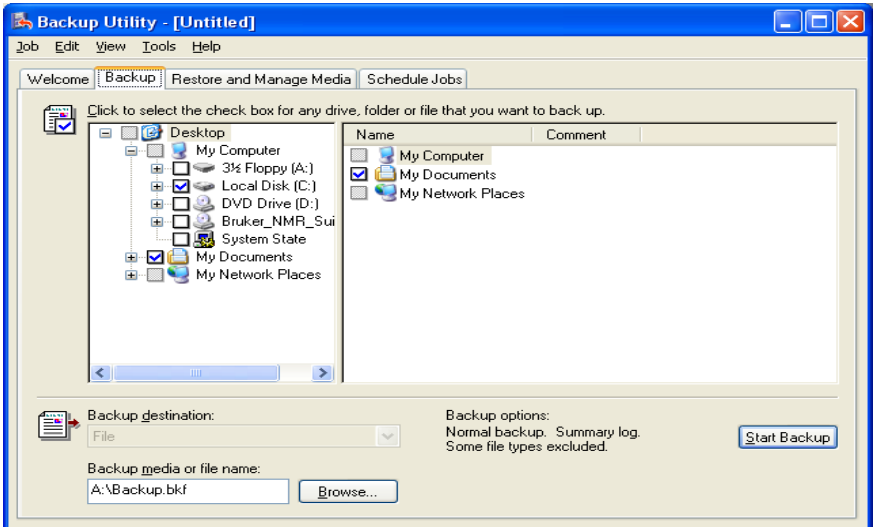
15.11.2 Backup of specific directories

1. Click **Start** → **All Programs** → **Accessories** → **System Tools** → **Backup**
   → a window *backup* will appear
2. Click **Backup**
   → all available drives will appear
3. Choose the directory you want to backup. Click the check box left of the directory to select the entire path for backup → a tick will appear in the check box
4. Choose the *Backup media or file*
5. Click **Start Backup**
6. A window *Backup Job Information* will open
7. Click **Start Backup**

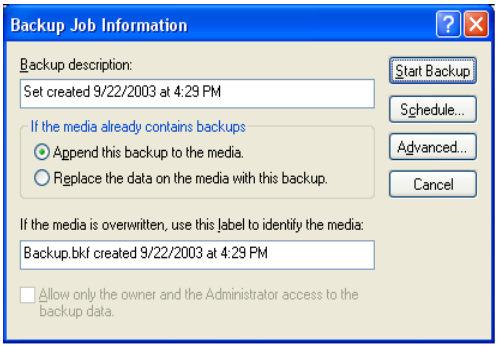
15.11.3 Frequent backup of specific directories

If you commonly use Ntbackup to back up a single folder, you might want to create a simple batch file. Suppose you would like to make a daily backup of a directory:

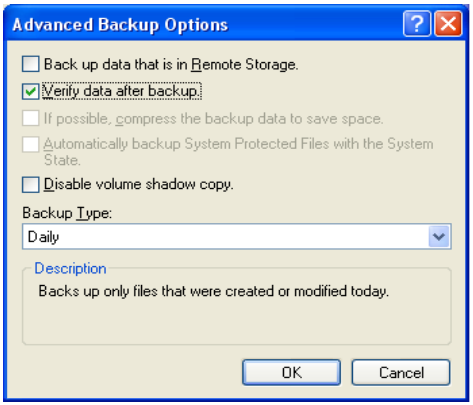
1. Choose the path of the file as describe above
2. Click **Start Backup**



3. A window *Backup Job Information* will open


Backup Job Information
Backup description:
Set created 9/22/2003 at 4:29 PM
If the media already contains backups
Append this backup to the media.
Replace the data on the media with this backup.
If the media is overwritten, use this label to identify the media:
Backup.bkf created 9/22/2003 at 4:29 PM
Allow only the owner and the Administrator access to the backup data.
Start Backup
Schedule...
Advanced...
Cancel

4. Click **Advanced**


Advanced Backup Options
Back up data that is in Remote Storage.
Verify data after backup.
If possible, compress the backup data to save space.
Automatically backup System Protected Files with the System State.
Disable volume shadow copy.
Backup Type:
Daily
Description
Backs up only files that were created or modified today.
OK
Cancel

5. Click the arrow at the right of the field *Backup Type* and choose **Daily**
6. Click **OK** → Click **Start Backup**

15.12 Security check of a Windows XP system

Microsoft offers a tool for free download that checks your PC for security leaks. The result is listed with an evaluation of the different topics. For further details check the following Microsoft website.

`http://www.microsoft.com/technet/treeview/default.asp?url=/technet/security/tools/Tools/mbsahome.asp`

15.13 Restore the Operating System to a Previous State in Windows XP

Use the System Restore tool in order to return your computer to a previous working state. The System Restore takes a 'snapshot' of critical system files and some program files and stores this information as 'restore points'. You can use these 'restore points' to return Windows XP to a previous state.

15.13.1 Using System Restore to Restore Windows XP

- **Windows XP Does Not Start**

  If Windows does not start, restart Windows by using the 'Last Known Good Configuration' feature:

  1. Start the computer and then press the **F8 key** when Windows begins to start. The 'Windows Advanced Options' menu appears.
  2. Select 'Last Known Good Configuration' (your most recent settings that worked), and then press **ENTER**.
  3. If a boot menu appears, use the ARROW keys to select **Microsoft Windows XP**, and then press **ENTER**. Windows XP restores the computer to the most recent restore point.

- **Windows XP Does Start**

  1. Log on to Windows as an administrator.
  2. Click **Start** → **All Programs** → **Accessories** → **System Tools** → **System Restore**. System Restore starts.
  3. A window *Welcome to System Restore* appears, click **Restore my computer to an earlier time** (if it is not already selected) → click **Next**.
  4. A window *Select a Restore Point* appears. Click the most recent system checkpoint in **On this list**, click a **restore point** list → click **Next**.
  5. A System Restore message may appear that lists configuration changes that System Restore will make → click **OK**.
  6. On the Confirm Restore Point Selection page, click **Next**. The System Restore will restore the previous Windows XP configuration and then restarts the computer.
  7. Log on to the computer as an administrator. A window *The System Restore*

Restoration Complete will appear → Click **OK**.

15.13.2 Troubleshooting

It could happen that you restore Windows XP to a previous configuration that you do not want. To undo the restoration:

1. Log on to Windows as an administrator.
2. Click **Start** → **All Programs** → **Accessories** → **System Tools** → **System Restore**. System Restore starts.
3. A window *Welcome to System Restore* appears. Click **Undo my last restoration** → **Next**.
4. A System Restore message may appear that lists configuration changes that System Restore will make → click **OK**.
5. On the **Confirm Restoration Undo** page, click **Next**. System Restore restores the original Windows XP configuration, and then restarts the computer.
6. Log on to the computer as Administrator. A window *The System Restore Undo Complete* appears → Click **OK**.

15.14 Turn on and turn off System Restore in Windows XP

The 'System Restore' is the feature that allows a computer system to be 'rolled back', or restored, to a point in time before certain events took place, for example, prior to specific software or hardware installations. System Restore monitors changes to the system and some application files, and automatically creates restore points. You can also create your own restore points at any time.

In Windows XP the 'System Restore' is enabled by default.

15.14.1 Turn on System Restore

To turn on System Restore, follow these steps:

1. Click **Start** → right-click **My Computer** → click **Properties**.
2. Click the **System Restore** tab.
3. Click to clear the **Turn off System Restore** check box (or the **Turn off System Restore on all drives** check box) → click **OK**.

15.14.2 Turn off System Restore

When you turn off System Restore, all existing restore points are removed, and you are no longer able to track or undo changes to your computer. To continue to use System Restore to restore your computer to a previous state, do not turn off System Restore.

To turn off System Restore, follow these steps:

1. Click **Start** → right-click **My Computer** → click **Properties**.
2. Click the **System Restore** tab.
3. Click to select the **Turn off System Restore** check box (or the **Turn off System Restore on all drives** check box) → click **OK**.
4. Click **Yes** when you receive the prompt to the turn off System Restore.

15.15 Start the system restore tool from a command prompt in Windows XP

Windows XP includes the System Restore tool, but you cannot start the System Restore tool from a Recovery Console prompt. Because of this, it may be useful to start the System Restore tool when you are unable to start your Windows XP-based computer normally or in Safe mode.

NOTE: You must log on with administrator rights.

1. Start your computer to Safe Mode with Command Prompt.
2. At the command prompt, type

   ```
   %systemroot%\system32\restore\rstrui.exe
   ```

   and then press ENTER.

   Follow the instructions on the screen to begin restoring your computer to a previous, functional state.

15.16 Logon problems: Last Known Good

Changes in the Registry must be made with extreme care, any mistakes can make the system unusable. Occasionally, software installations make erroneous Registry entries. If your PC does not boot any more, you can try to go back to the so-called

Last Known Good, the last Registry Control Set with which the system successfully booted. Please proceed as follows:

1. Reboot and Interrupt the boot process hitting F8 when you see:

   For troubleshooting and advanced startup of Windows XP press F8

2. Use the arrow down/up keys to select the entry *'Last Known Good'*, then press **ENTER** and follow the instructions

Warning: when you reboot the computer after you installed new software, wait until all disk activity has finished, before you log on. As soon as you log on, the current control set becomes the Last Known Good and the Original Control Set (before software installation) is gone.

15.17 Boot disks for Windows XP, if the CDROM is not bootable

If your computer does support booting from a CD-ROM, or if network-based installation is available, please use those installations methods instead.

The Windows XP startup disk allows computers without a bootable CD-ROM to perform a new installation of the operating system. Setup boot disks for Windows XP are available only by download from Microsoft. If you want to download the setup disks, the download contains only one large program file. When you execute the downloaded file, it extracts the files. There are six Windows XP Setup boot floppy disks, which contain the files and drivers that are required to access the CD-ROM drive and begin the setup process.

Note: You will need to use the Windows XP CD-ROM!

15.17.1 Downloading the Setup Disk Program File

To download the setup boot disks, please go to the Microsoft Web sites and download:

- Windows XP Professional Original Version

  http://www.microsoft.com/downloads/release.asp?ReleaseID=33291

- Windows XP Professional Service Pack 1 (SP1)

  Note: Windows XP CD-ROMs that include SP1 have the text "Includes Service Pack 1" on the CD-ROM.

  http://www.microsoft.com/downloads/release.asp?releaseid=42819

15.17.2 Creating the Setup Disks

Note: The program creates the setup boot disks for Microsoft Windows XP. To create these disks, you need to provide six blank, formatted, high-density disks.

1. Open the **Windows Explorer** and change to directory with the downloaded program file.
2. Double-click the *program file* (e.g. `WinXP_EN_PRO_BF.EXE` for Windows XP Professional Original Version).
3. A info window with the License Agreement appears: Click **Yes** to confirm.
4. A command prompt appears:

   This program creates the Setup boot disks for Microsoft Windows XP. To create these disks, you need to provide 6 blank, formatted, high-density disks.
   Please specify the floppy drive to copy the images to:
5. Enter the letter for the floppy disk drive (typically A).
6. After you typed in the floppy disk drive letter, you see the following message:

   Insert one of these disks into drive letter. This disk will become the Windows XP Setup Boot Disk.

   → Press any key when you are ready.
7. The file starts extracting and copying the files. Continue inserting the blank disks as you are prompted to do so until all six disks are created. If the process is interrupted you must run the downloaded program file again to create all six disks.

   Label each disk appropriately with the number that is specified by the program!

15.17.3 Using the Setup Disks

You have created all six disks:

1. Insert the first disk in the floppy disk drive → restart the computer.
   Note: The PC must be configured to boot from the floppy disk drive.
2. The setup process starts.
3. Insert the other floppy disks as you are prompted to do so.
   Note: You will need to use the Windows XP CD-ROM to finish Setup.

Chapter 16

File and directory handling

16.1 Viewing and opening files/directories

Windows XP offers three different ways of finding files or directories (folders). If you want to find a specific file and you have no idea where it resides, you can use the **Search** program. If you want to get an overview over the directory tree(s), you can use **Windows Explorer** or **My Computer**.

16.1.1 Windows Explorer

The Explorer provides an overview over all drives, directories and files in a two paned window.

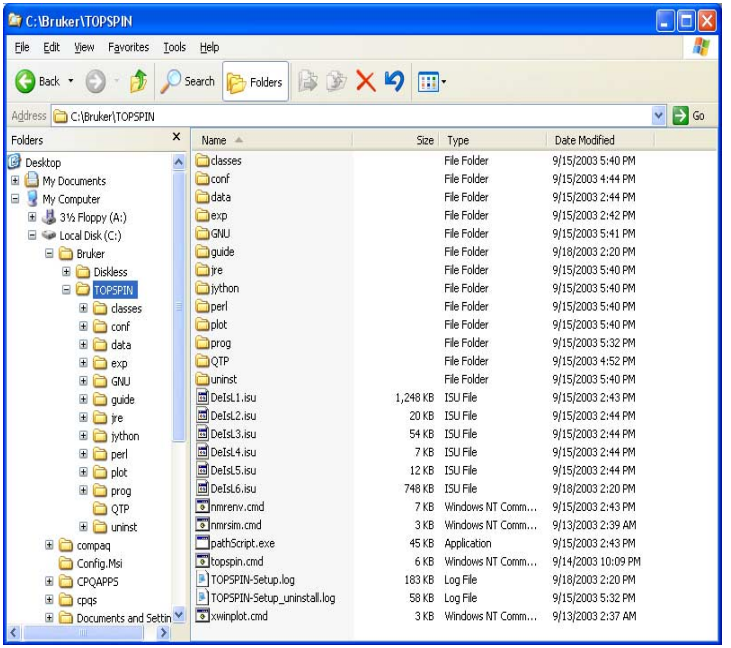
1. Click **Start** → **All Programs** → **Accessories** → **Windows Explorer**

   or right-click **Start** → **Explore**

2. A double-paned window '*Exploring*' appears
   - On the left side you see all drives and top level directories
   - On the right side you see the contents of the drive or directory which is currently selected on the left side.

A drive or directory can be expanded in the left pane by clicking on the '+' button to the left of its icon. The '+' button changes to a '-' button. When you click the

icon itself, contents of the directory will appear in the right pane. A double-click on the icon, both expands the directory and shows its contents


C:\Bruker\TOPSPIN
File Edit View Favorites Tools Help
Back Search Folders
Address C:\Bruker\TOPSPIN
Go
Folders
Desktop
My Documents
My Computer
3½ Floppy (A:)
Local Disk (C:)
Bruker
Diskless
TOPSPIN
classes
conf
data
exp
GNU
guide
jre
jython
perl
plot
prog
QTP
uninst
compaq
Config.Msi
CPQAPPS
cpqs
Documents and Settin
Name Size Type Date Modified
classes File Folder 9/15/2003 5:40 PM
conf File Folder 9/15/2003 4:44 PM
data File Folder 9/15/2003 2:44 PM
exp File Folder 9/15/2003 2:42 PM
GNU File Folder 9/15/2003 5:41 PM
guide File Folder 9/18/2003 2:20 PM
jre File Folder 9/15/2003 5:40 PM
jython File Folder 9/15/2003 5:40 PM
perl File Folder 9/15/2003 5:40 PM
plot File Folder 9/15/2003 5:40 PM
prog File Folder 9/15/2003 5:32 PM
QTP File Folder 9/15/2003 4:52 PM
uninst File Folder 9/15/2003 5:40 PM
DeIsL1.isu 1,248 KB ISU File 9/15/2003 2:43 PM
DeIsL2.isu 20 KB ISU File 9/15/2003 2:44 PM
DeIsL3.isu 54 KB ISU File 9/15/2003 2:44 PM
DeIsL4.isu 7 KB ISU File 9/15/2003 2:44 PM
DeIsL5.isu 12 KB ISU File 9/15/2003 2:44 PM
DeIsL6.isu 748 KB ISU File 9/18/2003 2:20 PM
nmrenv.cmd 7 KB Windows NT Comm... 9/15/2003 2:43 PM
nmrsim.cmd 3 KB Windows NT Comm... 9/13/2003 2:39 AM
pathScript.exe 45 KB Application 9/15/2003 2:43 PM
topspin.cmd 6 KB Windows NT Comm... 9/14/2003 10:09 PM
TOPSPIN-Setup.log 183 KB Log File 9/18/2003 2:20 PM
TOPSPIN-Setup_uninstall.log 58 KB Log File 9/15/2003 5:32 PM
xwinplot.cmd 3 KB Windows NT Comm... 9/13/2003 2:37 AM

16.1.2 My Computer

The **My Computer** window provides an overview over all drives, directories and files. The differences under Windows XP between the **Explorer** and **My Computer** are very small. In fact you can use both windows with the same layout and handling.

1. Double-click the icon **My Computer** on the desktop
2. A window *'My Computer'* will appear, showing the computer's drives:
3. Double-click a drive, e.g. (C:)
4. A window showing the contents of the top level directory on C: will appear:

   Double-click any icon. Depending on the file type, one of the following will happen:

   - A directory (Folder) will be opened and its contents will be shown

- An executable program will be started
- A text file will be opened using an editor (by default **`notepad`**)
- For an unknown file type, a window '*Open with*' will appear, showing a list of available programs

If you click a directory icon two things might happen:

- the directory contents appears in a new window
- the directory contents replaces the contents of the current window

You can configure this feature according to your preference:

a) Double-click the icon **My Computer** on the desktop

b) Click **Tools** → **Options**

c) A window '*Options*' will appear:

- Click **General** and select one of the two **options** of '*Browse Folders*'

The disadvantages of a separate window for each directory is that your screen is soon filled up with windows. However, a quick way of closing an entire hierarchy of windows is the key combination **ALT+SHIFT+F4**.

If you want the explorer layout as a two paned window, select **View** → **Explorer Bar** and enable '**Folders**'. You are not able to store this configuration, this might be the biggest difference between the **Explorer** and **My Computer**

16.1.3 Explorer and My Computer can hide file extensions

Windows XP Explorer and My Computer allow you to hide known file extensions like `.txt`, `.fm`, `.doc` etc. One of the problems when you hide them is that the editor Notepad appends the extensions `.txt` to files which do not have a known extension. For example, `license.dat` is changed to `license.dat.txt` and thereby becomes unusable. Therefore, we recommend to configure My Computer such that it shows file extensions:

1. Double-click **My Computer**
2. Click **Tools** → **Folder Options** → **View**
3. Unselect **Hide file extensions for known file types**
4. Click **OK**

This setting also applies to Explorer.

16.1.4 Search

The Windows XP Find program allows you to search files and directories according to various criteria.

Suppose you are looking for the file named `cosy`:

a) Click **Start** → **Search** → **For Files or Folders**

(or press **F3** when the cursor is on the desktop background)

b) Click the small arrow right of the field **Look in**: select the drive on which you expect to find the file. If you select **My Computer**, all drives will be searched.

c) In the field **Named**: enter `cosy`

d) Click **Find now**

All files which contain the string `cosy` in their name will appear in the result, e.g. `cosy`, `cosygs`, `pecosy`. You can directly open the file by clicking on it. Furthermore, you can also search for text files which contain a certain string if you define it in the field '*Containing Text*'. Clicking on '**Search Options**' will show you some more parameters like '*Date*' or '*Size*' which you can added in your search options

16.1.5 The Windows Command Prompt

A Windows XP Command Prompt (shell) can be opened in three ways:

- Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
- Click **Start** → **Run** enter **`cmd`** click **OK**
- Press **CTRL+ESC** → **`r`** enter **`cmd`** click **OK**

A window will appear where you can enter Windows commands like **`cd, dir, type, copy, ren, move, notepad, print, ipconfig, cacls, telnet, ftp`** etc.

The default Prompt is **C:\>** when the computer was booted from this drive.

16.2 File and directory permissions

Windows XP supports file level security on NTFS but not on FAT filesystems. Note that TOPSPIN can only be installed on NTFS and as such it supports file level

security.

16.2.1 Permissions and Types of Access

Folders and files can have the following permissions:

Permission	Full Control	Modify	Read & Execute	List Folder Contents[1]	Read	Write
Traverse Folder[1] / Execute File[2]	**yes**	**yes**	**yes**	**yes**	**no**	**no**
List Folders[1] / Read Data[2]	**yes**	**yes**	**yes**	**yes**	**yes**	**no**
Read Attributes	**yes**	**yes**	**yes**	**yes**	**yes**	**no**
Read Extended Attributes	**yes**	**yes**	**yes**	**yes**	**yes**	**no**
Create Files[1] / Write Data[2]	**yes**	**yes**	**no**	**no**	**no**	**yes**
Append Data	**yes**	**yes**	**no**	**no**	**no**	**yes**
Write Attributes	**yes**	**yes**	**no**	**no**	**no**	**yes**
Write Extended Attributes	**yes**	**yes**	**no**	**no**	**no**	**yes**
Delete Subfolders and Files	**yes**	**no**	**no**	**no**	**no**	**no**
Delete	**yes**	**yes**	**no**	**no**	**no**	**no**
Read Permissions	**yes**	**yes**	**yes**	**yes**	**yes**	**yes**
Change Permissions	**yes**	**no**	**no**	**no**	**no**	**no**
Take Ownership	**yes**	**no**	**no**	**no**	**no**	**no**
Synchronize	**yes**	**yes**	**yes**	**yes**	**yes**	**yes**

[1] folder permission

[2] file permissions

16.2.2 Changing file permissions

The permissions of a single file can be changed as follows:

1. Find the file in the Explorer (see chapter 16.1.1)

2. Right-click the file icon

3. Click **Properties**

4. A window '*Properties*' will appear:[1]

- Click **Security**

5. Highlight the user/group for whom/that you want to change the permissions

6. Click **Allow** or **Deny** to set the permissions

7. If you want to add a new user/group click on **Add**

8. A window '*Select Users, Computers or Groups*' will appear:

a) Select the one you are looking for **Add** → **OK**

9. Select the permissions you want to give to the new name

If you want to select special permissions, do step 1-5 then click **Advanced**

1. A window '*Access Control Settings for <filename>*' will appear:

- Click **Permissions** → **View/Edit**

2. A window '*Permission Entry for <filename>*' will appear:

- Click **Allow** or **Deny** of the permissions you want **OK** → **OK** → **OK**

16.2.3 Changing directory permissions

The permissions of a directory can be changed in the same way as file permissions:

In the window '*Permissions Entry for <directoryname>*' you can select in the Field '*Apply onto*' the effects of changing the permissions. Click the small arrow right of the field **Apply onto** and select the entry of your choice. You can select any combination between folder and/or subfolder and/or files **OK** → **OK** → **OK**

1. If Windows XP is installed the security section might be not displayed. If you like to see it, you have to define it in the options of Windows Explorer. Click on '**Tools**' → '**Folder Options**', click on '**View**' and disable the entry: '*Use simple file sharing (Recommended)*'

16.2.4 Read-only attribute

The problem of setting the **Read-only** attributes only in the entire directory and not in the subdirectory is solved under Windows XP:

1. Find the file or directory in the Explorer
2. Right-click its icon
3. Click **Properties**
4. A window '*Properties*' will appear:
   a) Click the attribute **Read-only** to switch it on or off
5. A window '*Confirm Attribute Changes*' will appear where you are able to decide if your changes are set only for the entire directory or also for the subdirectories and folders.

16.3 Known Problems in TOPSPIN for Windows XP

AU programs which were copied from another computer are sometimes not displayed properly by Notepad. This happens if they were transferred with FTP in binary mode. You can either transfer the file again using `ftp` in ascii mode or with `rcp` or you can correct the local AU program as follows:

1. **Start → All Programs → Bruker TOPSPIN → GNU Shell**
2. `vi au_program`

   in the editor window enter:

   ```
   :set textmode
   :wq!
   ```

3. `notepad au_program`

   → the AU program should be displayed correctly now

16.4 Compressing files and directories

16.4.1 Setting the Compress attribute

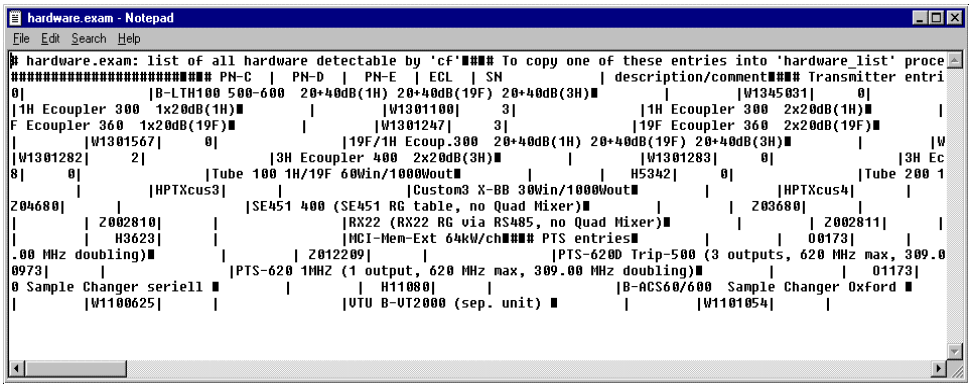
For each file and directory under Windows XP, you can set so called attributes. One of these is the Compress attribute which reduces the size considerably.

1. Right-click a file or folder in the Explorer
2. A popup menu will appear:
   - Click **Properties**
3. A window '*<name> Properties*' will appear:
   a) Click **Advanced**
   b) Enable the attribute **Compress Contents to save disk space → OK → OK**

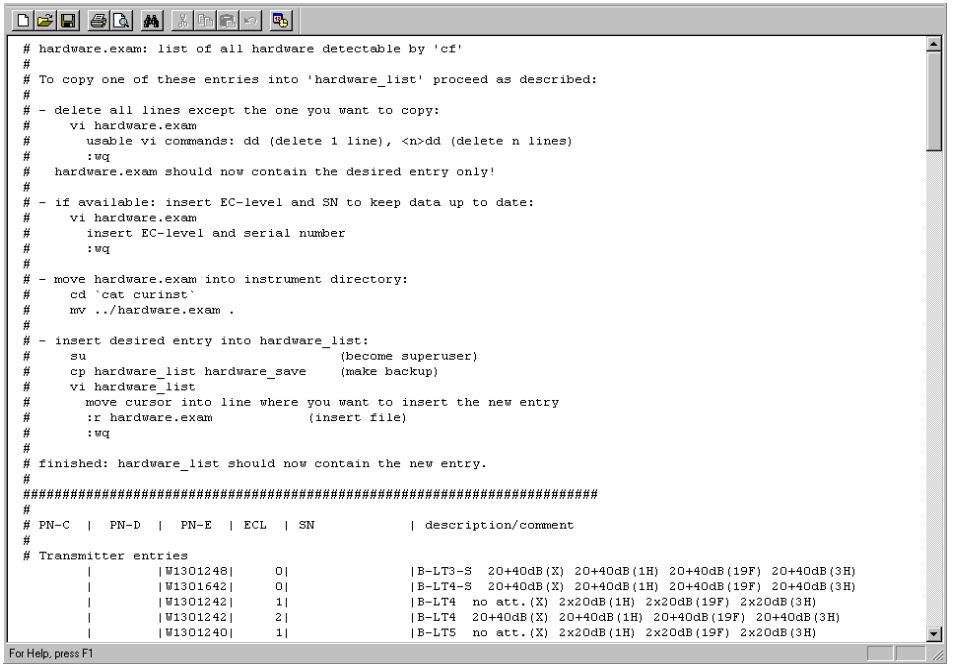
Compressed data will be uncompressed and recompressed automatically whenever they are accessed by an application. Note that this process will take time and your application runs slower when they work on compressed data. For transferring files or directories you might want to compress/archive them in zip format using the program Winzip rather than using the Compress attribute (see chapter 19.2).

16.5 Editing text files

You might know, UNIX doesn't write Carriage Returns (CR) at the end of text lines. That means that some files we create will not display properly in an editor like Notepad:


hardware.exam - Notepad
File Edit Search Help
hardware.exam: list of all hardware detectable by 'cf'### To copy one of these entries into 'hardware_list' proce
########################## PN-C | PN-D | PN-E | ECL | SN | description/comment### Transmitter entri
0| |B-LTH100 500-600 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)■ | |W1345031| 0|
|1H Ecoupler 300 1x20dB(1H)■ | |W1301100| 3| |1H Ecoupler 300 2x20dB(1H)■ |
F Ecoupler 360 1x20dB(19F)■ | |W1301247| 3| |19F Ecoupler 360 2x20dB(19F)■
| |W1301567| 0| |19F/1H Ecoup.300 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)■ | |W
|W1301282| 2| |3H Ecoupler 400 2x20dB(3H)■ | |W1301283| 0| |3H Ec
8| 0| |Tube 100 1H/19F 60Win/1000Wout■ | | H5342| 0| |Tube 200 1
| |HPTXcus3| | |Custom3 X-BB 30Win/1000Wout■ | |HPTXcus4| |
Z04680| | |SE451 400 (SE451 RG table, no Quad Mixer)■ | | Z03680| |
| | Z002810| | |RX22 (RX22 RG via RS485, no Quad Mixer)■ | | Z002811| |
| | H3623| | |MCI-Mem-Ext 64kW/ch### PTS entries■ | | 00173| |
.00 MHz doubling)■ | | Z012209| | |PTS-620D Trip-500 (3 outputs, 620 MHz max, 309.0
0973| | |PTS-620 1MHZ (1 output, 620 MHz max, 309.00 MHz doubling)■ | | 01173|
0 Sample Changer seriell ■ | | H11080| | |B-ACS60/600 Sample Changer Oxford ■
| |W1100625| | |VTU B-VT2000 (sep. unit) ■ | |W1101054| |

That doesn't mean that the file is damaged, it only means that the editor cannot resolve the issue. One reason to pick `WordPad` as an editor is that `WordPad` (unlike `Notepad`) is smart enough to render such files:



```
# hardware.exam: list of all hardware detectable by 'cf'
#
# To copy one of these entries into 'hardware_list' proceed as described:
#
# - delete all lines except the one you want to copy:
#     vi hardware.exam
#       usable vi commands: dd (delete 1 line), <n>dd (delete n lines)
#       :wq
#   hardware.exam should now contain the desired entry only!
#
# - if available: insert EC-level and SN to keep data up to date:
#     vi hardware.exam
#       insert EC-level and serial number
#       :wq
#
# - move hardware.exam into instrument directory:
#     cd `cat curinst`
#     mv ../hardware.exam .
#
# - insert desired entry into hardware_list:
#     su                                (become superuser)
#     cp hardware_list hardware_save    (make backup)
#     vi hardware_list
#       move cursor into line where you want to insert the new entry
#       :r hardware.exam            (insert file)
#       :wq
#
# finished: hardware_list should now contain the new entry.
#
##############################################################################
#
# PN-C  |  PN-D  |  PN-E  | ECL  | SN            | description/comment
#
# Transmitter entries
        |        |W1301248|     0|               |B-LT3-S  20+40dB(X) 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)
        |        |W1301642|     0|               |B-LT4-S  20+40dB(X) 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)
        |        |W1301242|     1|               |B-LT4  no att.(X) 2x20dB(1H) 2x20dB(19F) 2x20dB(3H)
        |        |W1301242|     2|               |B-LT4  20+40dB(X) 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)
        |        |W1301240|     1|               |B-LT5  no att.(X) 2x20dB(1H) 2x20dB(19F) 2x20dB(3H)
For Help, press F1
```

Thus, if you see displays like the Notepad-example above, please try a smarter editor: WordPad comes with every Windows and those that have Microsoft Word can of course use Microsoft Word to edit files in luxury.

16.6 Upper/Lower case letters

The Windows file system NTFS intentionally does not differentiate between upper and lower case letters. Therefore working on a PC, please observe the following:

1. if you want to work with your SGI spectra on a PC avoid to create datasets with the same name differentiated only by being written in upper or lower case letters.
2. do not ignore the upper and lower case letters of TOPSPIN commands. If for instance you type ***rpar PROT**** TOPSPIN will display the rpar-list of all parameter sets beginning with 'PROT'. The command ***rpar Prot**** will show no parameter list, although the MS-Explorer displays the parameter set 'PROTON' in the wrong way 'Proton'.

Chapter 17

Plotting and Printing under Windows XP

17.1 Printing / plotting data

17.1.1 Plotting and printing

Under Windows XP, all common printer drivers are available and printers are installed with the Windows XP **add printer** tool (see chapter 14.1). When a printer is installed under Windows XP, it can be used for plotting from TOPSPIN and TOPSPIN PLOT EDITOR.

The default printer and plotter for TOPSPIN are defined during the configuration of TOPSPIN by **expinstall** (see chapter 8.1.1).

17.1.2 Print/Plot from the Menu

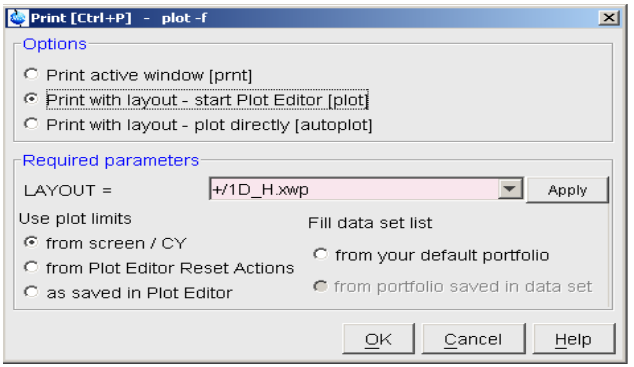
The current data window can be printed as follows:

1. From the TOPSPIN menu:

- Click the print button in the upper toolbar
- or Click **File** → **Print**

- or Enter ***print*** or ***Crtl-p***

All these actions are equivalent; they open the Print dialog box.



2. In the Print dialog box:

a) Select ***Print active window [prnt]***

b) Click ***OK***

Before printing starts, the operating system print dialog box will appear to select e.g. the printer and printer properties.

The Print dialog box contains two further options:

- ***Print with layout - start Plot Editor [plot]***

  If you select this option and click OK, the Plot Editor will be started. This option is equivalent to entering plot on the TOPSPIN command line.

- ***Print with layout - plot directly [autoplot]***

  Selecting this option activates the Plot Editor layout list box. Select the desired layout and click ***OK*** to print. Standard layouts are delivered with TOPSPIN. They use the Windows default printer. User defined layouts use the printer defined in the TOPSPIN PLOT EDITOR. On a 1D dataset, only 1D layouts are listed, on a 2D dataset only 2D layouts are listed etc.

For the last two options, the following Required Parameters are available.

Use plot limits:

- ***from screen/ CY***

  The plot limits and maximum intensity are used as they are on the screen (processing parameter F1P, F2P and CY, respectively)

- ***from Plot Editor Reset Actions***

  The plot limits and maximum intensity are set according to the TOPSPIN PLOT EDITOR Reset Actions (right-click inside the TOPSPIN PLOT EDITOR data field and choose Automation to set the Reset Actions).

- ***as saved in Plot Editor***

  The plot limits and maximum intensity are set in the specified layout

Fill dataset list:

- ***from your default portfolio***

  The portfolio contains the current TOPSPIN dataset plus the data from the default Plot Editor portfolio

- ***from port folio saved in dataset***

  The portfolio contains the current TOPSPIN dataset plus the data from the portfolio stored in this dataset

17.1.3 Plot data from the Processing guide

Printing/plotting data can be done from the Processing guide by clicking the ***Plot/Print*** button. If ***Automatic mode*** is checked, the active data window will be printed as it appears in the screen. If ***Automatic mode*** is unchecked, you will get the dialog box.

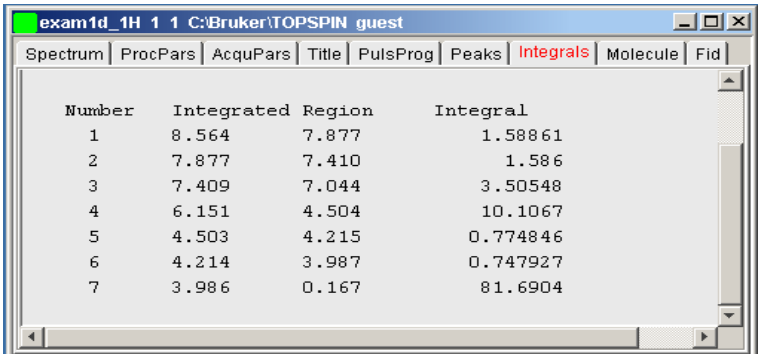
17.1.4 Plot data with the TOPSPIN PLOT EDITOR

Although the ***print*** command allows you to use or start the TOPSPIN PLOT EDITOR, you can also start it from the command line (enter ***plot***). This will open the TOPSPIN PLOT EDITOR from which you can create layouts and plot data. The complete TOPSPIN PLOT EDITOR functionality is described in its online manual that can be opened from the TOPSPIN PLOT EDITOR Help menu.

17.1.5 Print the Integral list

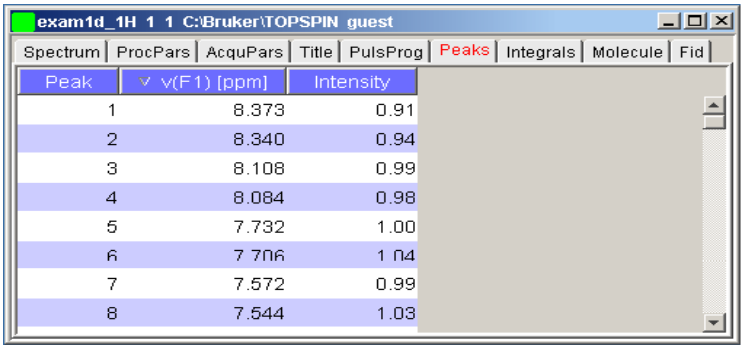
1. Click the Integrals tab of the data window

2. Enter ***print*** or ***Ctrl+p*** to print it


exam1d_1H 1 1 C:\Bruker\TOPSPIN guest
Spectrum ProcPars AcquPars Title PulsProg Peaks Integrals Molecule Fid
Number Integrated Region Integral
1 8.564 7.877 1.58861
2 7.877 7.410 1.586
3 7.409 7.044 3.50548
4 6.151 4.504 10.1067
5 4.503 4.215 0.774846
6 4.214 3.987 0.747927
7 3.986 0.167 81.6904

17.1.6 Print the Peak list

1. Click the Peaks tab of the data window
2. Enter ***print*** or ***Ctrl+p***



17.1.7 Copy data to Other Applications

Under Windows XP, you can easily copy the data window contents to other applications. To do that:

- Click **Edit** → **Copy** [copy]

This will copy the data window contents to:

- the clipboard. After that you can paste the clipboard contents to any Windows application.

- the Windows Metafile file screenDump.wmf in the user properties directory (enter ***hist*** to locate this directory). The Windows Metafile can be imported by other applications or send to a different computer.

Note: Some programs, when importing spectra from the clipboard or metafile, do not display the contained information correctly. Particularly when you resize the imported graphics, sections of the text, the spectrum, or the axis sometimes have disappeared.Usually this is only a display problem. When you print the respective page, the representation is correct.

17.1.8 Store (Export) a Data Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this, TOPSPIN allows you to save the contents of a data window in a graphics file of selectable type, e.g. .png, .tif, .wmf etc. To do that:

1. Click **Edit** → **Export**
2. Navigate to the storage folder
3. Enter the destination filename and extension
4. Click ***Export***

The resolution of such a screen dump equals the resolution of your screen. When you import a graphics file into an other program, you may loose information when resizing the graphics.

17.1.9 TOPSPIN PLOT EDITOR

1. TOPSPIN PLOT EDITOR uses the printer driver system of Windows XP for any printer output. This means that any printer for which a windows driver is correctly installed can be selected as print device. Note that the printer name in a layout file written by the Windows XP version is probably not known by the UNIX version of TOPSPIN PLOT EDITOR because of the different printer handling. Apart from that, layout files can be freely interchanged between the two platforms.
2. TOPSPIN PLOT EDITOR uses the Windows XP Clipboard. If you put one or more TOPSPIN PLOT EDITOR objects to the clipboard then these are stored in windows metafile format. Therefore any windows application which is able to read metafile data from the clipboard can import TOPSPIN PLOT EDITOR objects.

3. Another way of exporting graphics is the menu option '*File/Export*' which allows you to save the complete layout in Windows Enhanced Metafile format (EMF). Most current graphical-oriented windows applications can import this format. This provides a convenient way of importing TOPSPIN PLOT EDITOR graphics into programs like Word or Powerpoint.
4. With the TOPSPIN PLOT EDITOR you can directly send your current plot as Email. Just click **File** → **Send** and TOPSPIN PLOT EDITOR will pop-up your default mail client and add the current plot as an EMF attachment.

Chapter 18

Windows XP commands

18.1 Important Windows XP functions and their shortcuts

The following Windows XP functions will be used regularly in this manual. They can all be started in different ways by mouse click or by entering a command on the keyboard. The following section describes some ways to start important functions:

1. Open the **Management Console**:
   - **My Computer** → right click **Manage**
2. Working as other User:
   - Right click on many icons → choose **Run as ...**
   - Right click in Explorer on many applications → choose **Run as ...**
   - Type in a command prompt:

     runas /user:administrator cmd.exe

     this will ask you for the administrator password and then open a Command prompt with administrator permissions
3. Open the Control Panel:
   - Click **Start** → **Control Panel**

- Click **My Computer** → **Control Panel**
- Press **Ctrl+Esc** → **s** → **c**

4. Open a Command Prompt:
   - Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
   - Press **Ctrl+Esc** → **r** → enter **cmd** → click **Enter**
5. Open the Task Manager:
   - Click the RIGHT mouse button on the Taskbar → click **Task manager**
   - Press **Ctrl+Shift+Esc**
6. Search for files or directories:
   - Click **Start** → **Search** → **For Files or Folders**
   - Enter **Ctrl+Esc** → **s** → **s** → click **Enter**
   - Press **F3** while the focus is on the desktop

     (if the focus is not on the desktop: click on the desktop first)
7. Start the Windows Explorer:
   - Click **Start** → **All Programs** → **Accessories** → **Windows Explorer**
   - Right-click **Start** → **Explorer**
   - Double-click icon **My Computer** on the desktop
8. Configure the network:
   - Click **Start** → **Control Panel** → **Network Connections**
   - Right-click **My Network Places** → **Properties**
9. Close a hierarchy of windows opened from **My Computer**:
   - Press **Alt+Shift+F4**

More shortcuts may be found in chapter 18.3.1

Chapter 21.1 contains a blank list for important names and numbers of the hard- and software of your PC. It is recommended that you fill in the information there before you start the installation.

18.2 Online Help

Windows XP online help provides you with two kinds of help:

- help on specific topics
- help on what you see on your screen

18.2.1 Getting Help on specific topics

Click **Start** → **Help** (for a list of help topics)

- Click **Index** to get help on a predefined list of keywords
  - Enter the first letter(s) of a keyword
- Click **Find** to get help on all keywords contained in a data base

From the window which displays the help text you can go back to the main Help window by clicking **Help Topics**.

18.2.2 The question mark (?) in the upper right corner

Several windows, e.g. most windows which are opened from the Control Panel, have a question mark in the upper right corner. If you click it, the cursor will change to an arrow with a question mark. Now you can click a button or field you want information about. The information will disappear when you click the desktop background.

18.2.3 Tips on Windows XP

This window appears every time you log in, unless you unselect

Show this screen at startup

If you want this window back: click **Start** → **Run** enter `welcome` click **OK**

Click in the right window to read some tips.

18.2.4 Windows XP tips and tricks on the Web

Innumerous tips and tricks on Windows XP can be found on various Web pages.

18.3 Keyboard shortcuts

18.3.1 General Shortcuts

Function or mouse equivalent	Keyboard shortcut 1
Start	**CTRL+ESC**
Start → Documents	**CTRL+ESC d**
Start → Help	**- CTRL+ESC h** - **F1** from desktop or explorer
Start → Run	**- CTRL+ESC r** - **WIN+R**
Start → Search	**- CTRL+ESC c** - **F3** from desktop or explorer - **WIN+F**
Start → Shutdown	**CTRL+ESC u**
Taskbar → Task Manager	**CTRL+SHIFT+ESC**
Close the active window	**ALT+F4** [1]
Close a hierarchy of windows	**ALT+SHIFT+F4**
Switch to other task	**ALT+TAB**
Minimize all windows on desktop	**WIN+M**
Restore all windows as seen before	**WIN+SHIFT+M**
Toggle normal/full-screen Command Prompt	**ALT+ENTER**
Copy entire screen to Clipboard	**PRTSC** (Print Screen)
Copy active window to Clipboard	**ALT+PRTSC** (Print Screen)

1. Be careful: If no window is active Windows XP will prompt for reboot

18.3.2 Shortcuts for Windows Explorer

Function	Keyboard shortcut 1
Open new Explorer window	**WIN+E**
Rename file	**F1**
Open online help	**F2**
Open '*Find*' dialog	**F3**
Open '*Folder*' drop-down list	**F4**
Force refresh of windows contents	**F5**
Switch between left and right pane	**F6**
Go up one level in folder hierarchy	**BACKSPACE**
open context menu	**- SFHIFT+F10** - right mouse click

18.4 Command Prompt versus Graphical Interface

In a Windows environment, you normally work with a graphical interface, i.e. the **Start** button, Icons on the desktop, the Explorer etc. Nevertheless, Windows XP offers a Command Prompt, a shell, from which you can run various commands. The following table compares the Command Prompt with the graphical interface.

Function	Command Prompt	Graphical Interface
Files		
list files	`dir`	Explorer → Click **Drive** or **Folder**
delete a file	`del` (`erase`)	Right-click an icon in Explorer → **Delete**
rename a file	`ren`	Right-click an icon in Explorer → **Rename**
find text in files	`find`	**Start** → **Search** → **For Files and Folders** → **Containing text**

Function	Command Prompt	Graphical Interface
find a file		**Start → Search → For Files and Folders → Search for Files or Folders**
Directories		
make a dir.	`mkdir` (`md`)	**File → New → Folder**
remove a dir.	`rmdir`	Right-click icon in Explorer → **Delete**
change dir.	`cd <dir>`	Explorer
Utilities		
time and date	`date`, `time`	**Start → Settings → Control Panel → Date/Time**
backup	`ntbackup`	**Start → Programs → Accessories → System Tools → Backup**

18.5 Windows XP Command Prompt versus UNIX shell

Bruker BioSpin supports the TOPSPIN for both Linux and Windows XP. Here are some of the differences between these two operating systems which are of interest.

18.5.1 Directory specification

In a UNIX shell, pathnames are specified using the slash (/) character, whereas under Windows XP the backslash (\) character is used. Example:

UNIX shell: `cd /Bruker/TOPSPIN`

Windows XP Command Prompt: `cd \Bruker\TOPSPIN`

Under UNIX, command options are usually specified with a minus character (-) whereas in an Windows XP Command Prompt, the slash (/) character is used. For example, the command for listing files sorted by date:

UNIX shell: `ls -lrt`

Windows XP Command Prompt: `dir /od`

18.5.2 Windows XP commands versus UNIX commands

Under Windows XP, most commands can be executed via the Graphical Interface. You can, however, also open a Windows XP Command Prompt and run commands from there. Here is a list of UNIX shell commands and the corresponding Windows XP shell commands:

Function	UNIX shell	Windows XP Command Prompt
Files		
List files	`ls`	`dir`
copy a file	`cp`	`copy`
rename a file	`mv`	`ren`
delete a file	`rm`	`del` (`erase`)
print a file	`lp`	`print`
edit a file	`vi`, `jot`	`notepad`
display file contents	`cat`	`type`
sort a file	`sort`	`sort`
compare 2 files	`diff`	`comp`, `fc`
find text in file	`grep`	`find`
find a file	`find`	
Directories		
make a directory	`mkdir`	`mkdir`
remove a directory	`rmdir`	`rmdir`
copy a directory	`cp -r`	`xcopy`
change directory	`cd <dir>`	`cd <dir>`
show current directory	`pwd`	`cd`
Utilities		
time and date	`date`	`date`, `time`

Function	UNIX shell	Windows XP Command Prompt
manual pages	`man`	`help`
backup	`tar`	`backup` (`floppy`) or `ntbackup` (`tape`)

18.6 The UNIX GNU shell

For compatibility reasons, a UNIX shell is delivered on the TOPSPIN CD and automatically installed during the installation of TOPSPIN. When the installation is finished you can open a GNU shell by clicking:

Start → All Programs → Bruker TOPSPIN → GNU Shell

A GNU shell will open in which you can enter a restricted set of UNIX commands.

Chapter 19

Useful tools for Windows Windows XP

This chapter contains a description of some tools we found useful. We realize that many other tools are available for various purposes and we are very interested in your experiences. Just send your comments to:

`nmr-software-support@bruker-biospin.de`

19.1 Update the operating system

There are two things that help you to be up-to-date with the operating system

- email notification about security fixes
- download and installation of hotfixes and service packs

Please see also chapter Microsoft Security Center (chapter 20.8).

19.1.1 Email notification about security fixes

Microsoft offers the possibility to subscribe for a newsletter that will inform you about security problems and their available fixes. Open Internet explorer and type in:

http://register.microsoft.com/regsys/pic.asp

You can subscribe there with your email address and after registration you can decide which kind of newsletter you want to get. It is recommended to subscribe at least for the *Microsoft Security Notification Service* to get all information about security leaks and their fixes.

19.1.2 Update of the operating system

- Click on **Start** → **All Programs** → **Internet Explorer Windows Update**
- The Internet Explorer will open. Click on **Tools** → **Windows Update**
  This will show a page where you can choose to start the search for all necessary updates.
- After the search is finished you have to choose which update of the available list you like to download.
- Start the download and follow the instructions.

19.2 Winzip: pack/unpack zip, tar, gz, uue files

The program Winzip allows you to pack or unpack archive files. The most common format is `.zip`, but Winzip also handles several other Windows and UNIX formats like `.tar`, `.gz` (created with gzip) and `.uue` (created with uuencode). An Evaluation Version of WinZip is available at: `www.winzip.com` which can be used for viewing and extracting archives. For creating archives, you should order an official version. Once Winzip is installed, it is automatically started when you click a file with the extension `.zip`, `.tar`, `.gz`, `.uue` etc. You can also drag and drop the file's icon into the Winzip window. Then click **Extract** to extract one file from the archive or click **Checkout** to extract all files.

19.3 Defragment your disk

Windows XP has an tool that allows you to defragment your disk. In the course of time your disk will become more and more fragmented. Although an NTFS partition (which is required for TOPSPIN), suffers much less from fragmentation than a FAT partition, it might be a good idea to defragment it from time to time.

Start → **All Programs** → **Accessories** → **System Tools** → **Disk Defragmenter**

Chapter 20

Windows XP Tips and Tricks

20.1 Creating shortcut icons on the desktop

20.1.1 Creating shortcut icons to programs

For frequently used programs, it is convenient to create a shortcut icon on the desktop. For example, a shortcut to the editor **`Notepad`** can be created as follows:

1. Right-click the **Start** button

2. Click **Open**

3. A window '*Start Menu*' will appear:

a) Click **All Programs** → Click **Accessories**

b) Press and hold the right mouse button on the **Notepad** icon

c) Drag the **Notepad** icon on the desktop, then release the right mouse button

d) Click **Create Shortcut(s) Here**

Alternatively, you can click **Start** → **Search** to find the executable file `Notepad.exe` and perform step c to d. (see also chapter 20.1.2).

20.1.2 Creating shortcut icons to documents/files:

For frequently used files, it is convenient to create a shortcut icon on the desktop. If Windows XP recognizes the extension of the file, the corresponding program to read the file will be started, e.g. Word for a `.doc` file. For a text file without extension, you can specify the program to be used. e.g. notepad, in the shortcut properties. As an example we will use the TOPSPIN history file:

1. Find the directory `<var>\prog\curdir\<user>` in the Explorer
   e.g. `C:\Bruker\TOPSPIN\prog\curdir\guest`
2. Press and hold the right mouse button on the icon **history**
3. Drag the **history** icon on the desktop, then release the right mouse button
4. Click **Create Shortcut(s) Here**
   → an icon Shortcut to `history` will appear
5. Right-click the icon **Shortcut to history**
6. Click **Properties**
7. A window '*Shortcut to history properties*' will appear:
   a) Click **Shortcut**
   b) In the field **Target**: insert the program to be used before pathname, e.g.
   notepad C:\Bruker\TOPSPIN\prog\curdir\guest\history
   c) Click **OK**

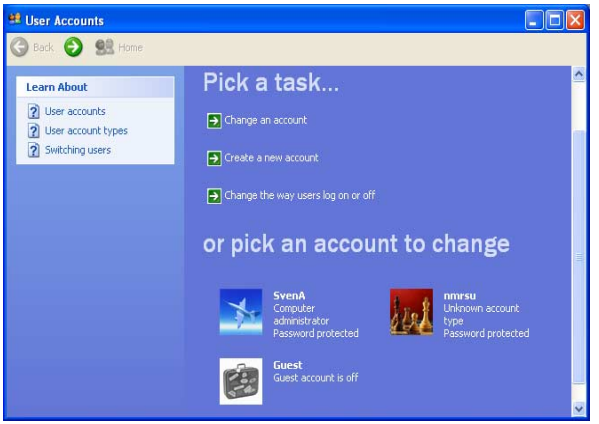
20.2 Use the classic logon screen under Windows XP

To temporarily use the classic logon screen, press CTRL+ALT+DEL two times on the Welcome logon screen.

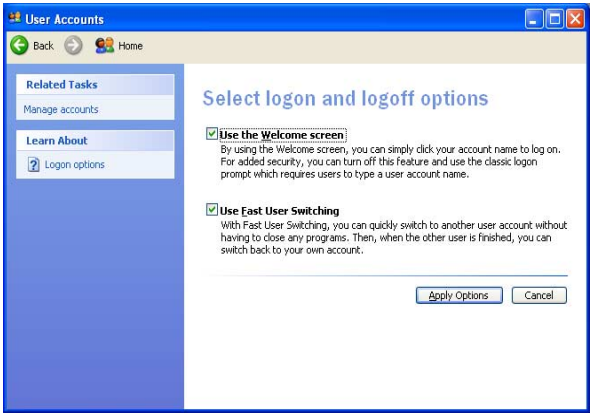
To configure Windows XP to use the classic logon and shutdown screens for every logon session, follow these steps:

1. Click Start, and then click Control Panel.
2. Double-click User Accounts.

3. Click Change the way users log on or off.



4. Clear the Use the Welcome screen check box.


User Accounts
Back
Home
Related Tasks
Manage accounts
Learn About
Logon options
Select logon and logoff options
Use the Welcome screen
By using the Welcome screen, you can simply click your account name to log on. For added security, you can turn off this feature and use the classic logon prompt which requires users to type a user account name.
Use Fast User Switching
With Fast User Switching, you can quickly switch to another user account without having to close any programs. Then, when the other user is finished, you can switch back to your own account.
Apply Options
Cancel

20.3 Convenient handling of TOPSPIN under Windows XP

20.3.1 Reading data from the Explorer into TOPSPIN

TOPSPIN can read data from the Explorer, via the Clipboard. Perform the following steps:

a) In the Explorer:

- Find the dataset you want to display in TOPSPIN

- Right-click the data name folder
- A popup window will appear: click **Copy**

b) In TOPSPIN:

- click ***File*** → ***Paste***

You can also click a data expno or procno folder and read the corresponding dataset into TOPSPIN.

20.3.2 Copy a text item into the TOPSPIN command line

Any text item which can be copied to the Clipboard can be pasted to the TOPSPIN command line. Of course this is only useful if this text item is an existing TOPSPIN command. You can, for example, copy an TOPSPIN command from the manual to the command line:

1. Click ***Help*** → ***Complete Processing Manual***
2. A PDF viewer (if installed) will start up showing the TOPSPIN processing manual:
   a) Click **Tools** → **Select text**
   b) Mark an TOPSPIN command in the manual, e.g. ***`search`***
   c) Enter **Ctrl-C**
3. Move the cursor on the TOPSPIN command line:
4. Click the middle mouse button.

This feature is especially useful for long command names or commands with many arguments.The text can come form various sources, e.g. online documents, the Command Prompt, text editors. You can, however, not copy file or program names directly from the Explorer to the TOPSPIN command line.

20.4 Various useful configurations

This paragraph describes several settings that we found useful. They have no influence on the TOPSPIN performance and you are free to choose your own settings.

20.4.1 Configuring the Taskbar

1. Right-click the Taskbar [1]

2. Click **Properties**
3. A window '*Taskbar Properties*' will appear:
   - De-select the item **Always on top**, click **OK**

This will create more space on the desktop.

20.4.2 Hide known file extensions

See chapter 16.1.3

1. Open the Explorer
2. Click the menu **Tools** → **Folder Options**
3. In the '*Folder Options*' window:
   a) Select **VIEW**
   b) Unselect **Hide file extensions for known file types** (if it is selected)
   c) Click **OK**

20.4.3 Show hidden files and folders

1. Open the Explorer
2. Click the menu **View** → **Options**
3. In the '*Folder Options*' window:
   a) Select **VIEW**
   b) Select **Show hidden files and Folders**
   c) Click **OK**

20.4.4 Configuring the GNU shell

The GNU shell is delivered on the CD '*TOPSPIN for Windows XP*' and is automatically installed together with the installation of TOPSPIN. It provides a set of UNIX commands. By default, the resize and cut & paste functions are not active.

Making the GNU window resizable by default:

1. Click **Start** → **All Programs** → **Bruker TOPSPIN** → **GNU Shell**
2. A GNU shell window will appear:

1. The taskbar is usually, but not necessarily, at the bottom of the screen

a) Click the symbol in the upper left corner of the window

b) Click **Properties**

3. A window '*GNU shell properties*' will appear:

a) Click **Layout**

b) In the field Screen Buffer Size:

- Set **Width** to 200
- Set **Height** to 100

c) Click **OK**

4. A window '*Apply properties to shortcut*' appears:

a) Click **Modify shortcut which started this window**

b) Click **OK**

Enabling the cut & paste function:

1. Click **Start** → **All Programs** → **Bruker TOPSPIN** → **GNU Shell**
2. A GNU shell window will appear:

a) Click the symbol in the upper left corner of the window

b) Click **Properties**

3. A window '*GNU shell properties*' will appear:

a) Click **Options**

b) Select **QuickEdit Mode**

4. A window '*Apply properties*' appears:

- Click **Apply properties to current window only**
- Click **OK**

The reason we do not recommend to enable the cut & paste function by default is that it would also count for the GNU shell started by TOPSPIN. Accidentally using cut & paste in that window could cause TOPSPIN to crash.

20.5 Connecting UNIX and Windows XP with Samba

Samba is a suite of programs which work together to allow clients to access UNIX file systems and printers via the SMB (Session Message Block) protocol.

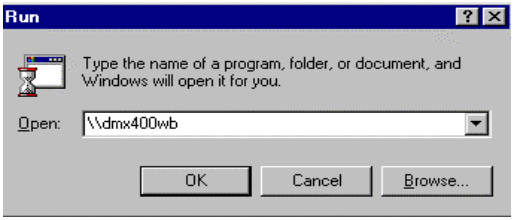
In practice, this means that you can 'share' disks and printers with UNIX systems. You can then access them from LanManager clients, Windows for Workgroups 3.11 clients, Windows95 clients, Windows NT clients, Windows 2000 clients, Windows XP clients and OS/2 clients. A 'share' is a term used to describe resources (directories, printers, etc.) that the server is making available for others on the network to use.

More information you may find in chapter 13.4.3, in the directory `/usr/samba/README` and `/usr/samba/docs` or if you have Internet access on `http://samba.org`

The license conditions are described in */usr/samba/COPYING*.

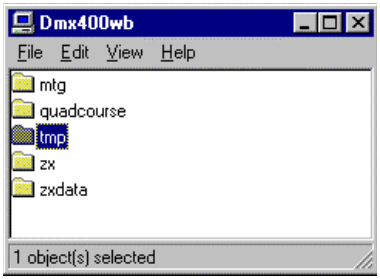
20.5.1 Accessing the network share provided by Samba

5. You can access shares from any Windows XP PC using the **Run**… feature available from the **Start** button.



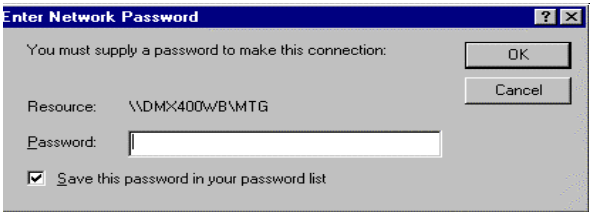
Type in two back-slashes followed by the (UNIX-)computer name (this operation is equivalent to running a '*find*' on a particular computer.

6. The corresponding response shows up in a Windows Explorer window:

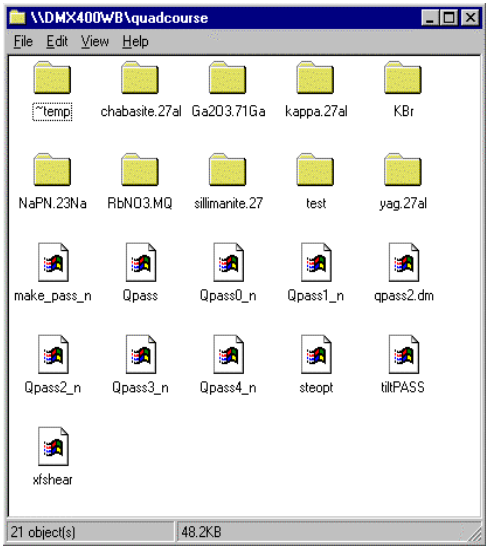


You can double-click on the share you want to see and it will come up with either a

password request for shares with managed access…



… or the list of contents (in yet another Explorer window):



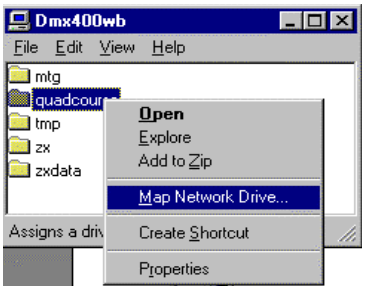
If you cannot get access to a share that you see and you are confident that the password is correct please see chapters 20.5.3 and 20.5.4.

To copy files you can drag-and-drop them from a content display and deal with files and directories as if they where local (e.g. you can drag-and-drop acqu-files into a Wordpad-icon on you desktop. Technically the job of making a connection is completed here.

20.5.2 Mapping network shares into 'local' drives

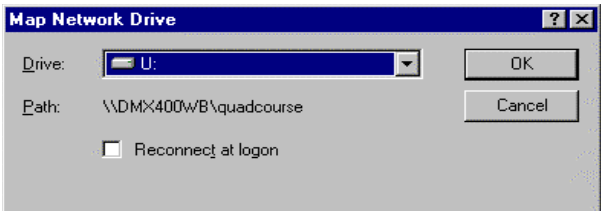
For some applications (including TOPSPIN) you will need, however, to map the network share to a (virtual) disk drive. That is: You create a look-alike of a local drive like, say, U: that points to the share you assign to it. Doing this is very simple:

Step #1: click with the right mouse button on the share you want to map to a disk drive

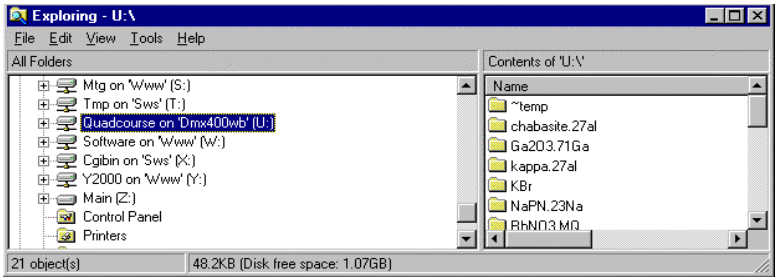


Select '**Map Network Drive**' (as shown).

Step #2: Select an appropriate drive letter (here: `U:`) and decide whether or not to click the '**reconnect at logon**' box. If you want a permanent connection that automatically is re-established any time the (client) PC is booting up click this box. If you don't check it this connection will only last until the next reboot.



Step #3: Press '**OK**'. As you press '**OK**' the system will connect this network share as a new drive called `U:` You can look up the new virtual disk in Windows Explorer after a few seconds:



On the right-hand side the files shared out from UNIX are shown and you can go about copying, moving etc just like with native Windows files.

20.5.3 *Configuring Windows XP to handle UNIX-style password requests*

One of the most annoying problems with SAMBA is that older versions are not able to authenticate network connectors using encrypted passwords. In SAMBA 2.0.x the default setting is still plain password but you could change it to encrypted. This is the best way for the security of your network. If you want to use the plain-text password, it is possible on Windows XP side, to enable the authentication with clear-text passwords sent over the networking enabling the respective registry key (see the following chapters 20.5.5 and 20.5.4)

NOTE THAT THIS INTRODUCES A SIGNIFICANT SECURITY LEAK!

20.5.4 Enable Plain Text Password

1. Log in as administrator.
2. Click **Start** → **Control Panel**
3. Click **Administrative Tools** → **Local Security Policy**
4. Enable the tree **Local Policies** → **Security Options**
5. On the right side double click the entry '**Send unencrypted password to ...**'
6. Click on '**enabled**'
7. If your computer is part of a Windows NT / 2000 / XP domain contact your domain administrator about this policy setting and its interaction with possible 'group policies'

20.5.5 There is one shortcut you can try with newer samba-versions

They deliver a file called `WinXP_PlainPassword.reg` in the `../samba/docs` directory. If you can locate this file in the Windows Explorer and double-click it, it will automatically make the additions to the registry file detailed hereafter. If you double-clicked the file and it worked you are done here. If not, you need to proceed as detailed in chapter 20.5.4 and manually make the necessary changes.

20.6 How to log on to Windows XP if you forget your password

20.6.1 Method 1: Log On as an Administrator and Reset the Password

If you can not log on to Windows by using a particular user account (including the Administrator or Computer Administrator accounts), but you can log on to another account with administrative privileges (including the Administrator or Computer Administrator accounts), follow these steps:

1. Log on to Windows by using the administrator account that has a password that you remember.

   Note: You cannot log on as usual by using the Administrator or Computer Administrator account to a Windows XP Professional-based computer in a workgroup. To log on as the Administrator or Computer Administrator, you must start Windows XP in Safe Mode.

2. Click **Start** → Click **Run**.
3. In the Open box, type the following command, and then click **OK**:

   ```
   control userpasswords2
   ```

4. Click the user account that you forgot the password for → Click **Reset Password**.
5. Type a new password in both the New password and the confirm new password boxes → Click **OK**.

You should now be able to log on to Windows with the user account and the new password.

WARNING: If you reset the password for a user account in this manner in Windows XP Professional, the following types of information for that user will be no longer available:

- E-mail messages that are encrypted with the user's public key
- Internet passwords that are saved on, or remembered by, the computer
- Any files that the user has encrypted

20.6.2 Method 2: Use a Password Reset Disk

If you created a password reset disk for Windows XP, you are able to reset your password by using the password reset disk. For additional information about how

to use a password reset disk, please check the articles in the Microsoft Knowledge Base:

- In order to create and use a Password Reset Disk for a computer that is not a domain member in Windows XP please read:

  `http://support.microsoft.com/default.aspx?scid=kb;EN-US;305478`

- In order to create and use a Password Reset Disk for a computer in a domain in Windows XP please read:

  `http://support.microsoft.com/default.aspx?scid=kb;EN-US;306214`

20.7 Error Message When You Use the Add Printer Wizard

When you create a printer (either a local printer or a remote network printer) by using the *Add Printer Wizard*, you may receive the following error message: "Operation could not be completed. The print spooler service is not running."

This error occurs because the Spooler service has not been started or has stopped working. To start the Spooler service, follow these steps:

1. Click **Start** → Click **Control Panel**.
2. Double-click **Administrative Tools** → Click **Services**.
3. Double-click the **Printer Spooler** service → Change the startup type to **Automatic**. This sets the Spooler service to start automatically when you restart the computer.
4. If you want to start the spooler service immediately, click the **Start** button under the **Service Status** field.

20.8 Microsoft Security Center

If you connect your computer to the Internet, you can be vulnerable to viruses, worms, hackers, and other Internet intruders. To help protect your computer against viruses and other security threats, Bruker BioSpin recommends to have a firewall and updated antivirus software running at all times.

Microsoft Windows XP Service Pack 2 (SP 2) contains the new Security Center, which helps you to manage your computer's security settings and therefore more

secure. If you are not running a firewall or an up-to-date version of antivirus software, you will see an alert in the notification area, to the right of the taskbar.

Wit the help of the Security Center you can check the status of the important security settings. You can also use it to find information about the latest virus or other security threat or to get customer support from Microsoft for a security-related issue.

20.8.1 How to open Security Center

1. Click **Start** → **Control Panel**.
2. Double-click **Security Center**. A window 'Microsoft Security Center' will appear:

Windows Security Center
Security Center
Help protect your PC
Resources
Get the latest security and virus information from Microsoft
Check for the latest updates from Windows Update
Get support for security-related issues
Get help about Security Center
Change the way Security Center alerts me
Security essentials
Security Center helps you manage your Windows security settings. To help protect your computer, make sure the three security essentials are marked ON. If the settings are not ON, follow the recommendations. To return to the Security Center later, open Control Panel.
What's new in Windows to help protect my computer?
Firewall
ON
Automatic Updates
ON
Virus Protection
ON
G DATA AntiWrenKit 2004 reports that it is up to date and virus scanning is on. Antivirus software helps protect your computer against viruses and other security threats. How does antivirus software help protect my computer?
Note: You now have antivirus software that Windows can monitor. Click Recommendations to find out how.
Recommendations...
Manage security settings for:
Internet Options
Automatic Updates
Windows Firewall

The Security Center helps to check that you have:

- A software firewall.
- Configure the settings for Automatic Updates.
- An up-to-date antivirus program.

If the Security Center detects that your computer might benefit from enhanced security in one of the three areas (Firewall, Automatic Updates and Antivirus program), it displays an alert in the notification area (to the right of the taskbar). An

alert message is displayed every time you log on, until the problem is fixed.

Windows Security Center checks for many common antivirus and firewall programs, but it is possible that you might be using a program that Windows can't find. If you are not sure about the status of your antivirus or firewall solution, or if you receive a Security Center alert that seems incorrect, check with your antivirus or firewall vendor to find out if the software you are running is supported in the Security Center.

Note: *If your computer is part of a domain, your security settings are typically managed by your network administrator. In this case, the Security Center does not display your security status or send alerts.*

20.8.1.1 What do the new security icons mean?

Windows XP SP2 contains a set of security icons that can help you recognize potential security risks and choose appropriate security settings.

These icons means:

- Indicates important security information and settings.
- Notifies you of a potential security risk.
- Situation is more secure. Your computer is using recommended security settings.
- Warning: situation is potentially harmful. Consider adjusting security settings to enhance the security of your computer.
- Your computer's current security settings are not recommended.

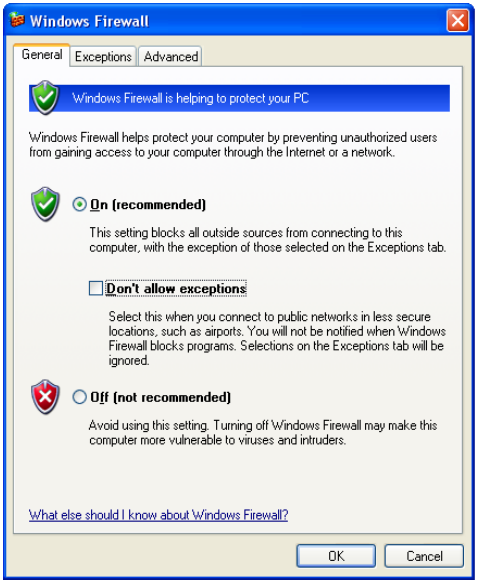
20.8.2 Firewall

Windows Firewall, previously known as Internet Connection Firewall or ICF, is a protective tool that monitors and restricts information that travels between your computer and a network or the Internet. This provides a line of defence against someone who might try to access your computer from outside the Windows Firewall without your permission.

Bruker BioSpin recommends to protect your computer against viruses or security threats, we recommend to keep the Windows Firewall (or another firewall) on.

20.8.2.1 To open Windows Firewall

1. Click **Start** → **Control Panel**.
2. In the window **Control Panel** → click **Windows Security Center**.
3. Click **Windows Firewall**.
4. A window 'Windows Firewall' appears:


Windows Firewall
General
Exceptions
Advanced
Windows Firewall is helping to protect your PC
Windows Firewall helps protect your computer by preventing unauthorized users from gaining access to your computer through the Internet or a network.
On (recommended)
This setting blocks all outside sources from connecting to this computer, with the exception of those selected on the Exceptions tab.
Don't allow exceptions
Select this when you connect to public networks in less secure locations, such as airports. You will not be notified when Windows Firewall blocks programs. Selections on the Exceptions tab will be ignored.
Off (not recommended)
Avoid using this setting. Turning off Windows Firewall may make this computer more vulnerable to viruses and intruders.
What else should I know about Windows Firewall?
OK
Cancel

Because a firewall restricts communication between your computer and the Internet, you might need to adjust settings for some programs that prefer an open connection. These adjustments are called 'exceptions'.

Windows Firewall now has three settings:

1. **On:** Windows Firewall is turned on by default, and normally you should leave it that way. When you choose this setting, Windows Firewall blocks all unsolicited requests to connect to your computer, except for requests to programs or services selected on the **Exceptions** tab.
2. **On with 'Don't allow exceptions':** When you select the **Don't allow exceptions** check box, Windows Firewall blocks all unsolicited requests to connect to

your computer, including requests to programs or services selected on the **Exceptions** tab. Use this setting when you need maximum protection for your computer (e.g. when you connect to a public network in a hotel or airport)

There is no need to keep **Don't allow exceptions** selected all the time, because when it is, some of your programs might not work correctly, and the following services are blocked from accepting unsolicited requests:

- File and Printer Sharing
- Remote Assistance and Remote Desktop
- Discovery of network devices
- Preconfigured programs and services on the exceptions list
- Additional items that you've added to the exceptions list

3. **Off:** This setting turns Windows Firewall off. When you choose this setting, your computer is much more vulnerable to harm from unknown intruders or viruses. This setting should only be used by advanced users for computer administration purposes, or if your computer is protected by another firewall.

20.8.2.2 Windows Firewall settings

If you are running Windows XP SP2 the Windows Firewall is turned on by default. This means that most programs will not be allowed to accept unsolicited communications from the Internet unless you choose to list those programs as exceptions. There are two programs that, by default, are already added to the exceptions list: **Files and Settings Transfer Wizard** and **File and Printer Sharing**.

Because firewalls restrict communication between your computer and the Internet, you might need to adjust settings for some other programs that prefer an open connection. You can make an exception for these programs, so that they can communicate through the Windows Firewall.

Each time you allow an exception for a program to communicate through Windows Firewall, your computer is made more vulnerable. If you have lots of exceptions and open ports, your computer can become more vulnerable. To help decrease your security risk:

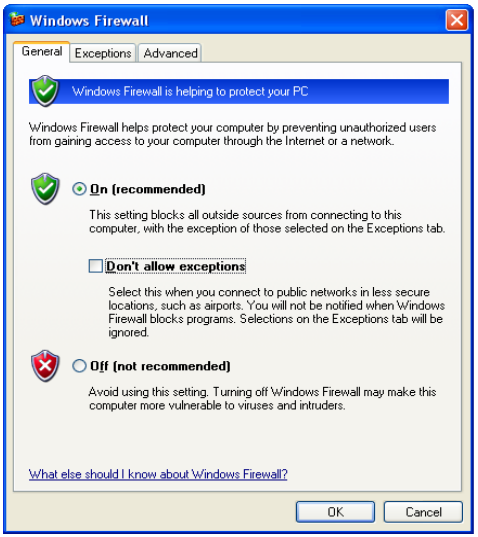
- Only allow an exception when you really need it.
- Never allow an exception for a program that you don't recognize.
- Remove an exception when you no longer need it.

Sometimes you might want someone to be able to connect to your computer, despite the risk such as when you expect to receive a file sent through an instant messaging program.

You can use the Bruker BioSpin `setfirewall.cmd` script to configure the Windows firewall (see chapter 8.8).

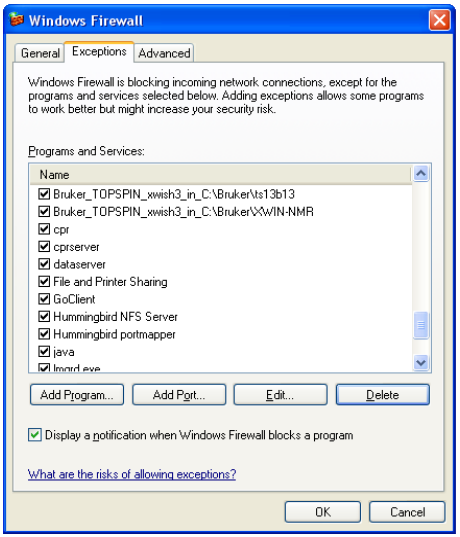
20.8.2.3 To add a program to the exceptions list

1. Click **Start** → **Control Panel**.
2. In the window **Control Panel** → click **Windows Security Center**.
3. Click **Windows Firewall**.
4. A window 'Windows Firewall' appears:.


Windows Firewall
General
Exceptions
Advanced
Windows Firewall is helping to protect your PC
Windows Firewall helps protect your computer by preventing unauthorized users from gaining access to your computer through the Internet or a network.
On (recommended)
This setting blocks all outside sources from connecting to this computer, with the exception of those selected on the Exceptions tab.
Don't allow exceptions
Select this when you connect to public networks in less secure locations, such as airports. You will not be notified when Windows Firewall blocks programs. Selections on the Exceptions tab will be ignored.
Off (not recommended)
Avoid using this setting. Turning off Windows Firewall may make this computer more vulnerable to viruses and intruders.
What else should I know about Windows Firewall?
OK
Cancel

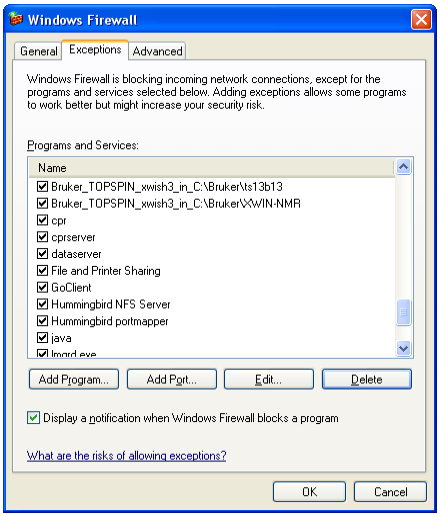
5. Click on the **Exceptions** tab. Under **Programs and Services**, select the check

box for the program or service that you want to allow, and then click **OK**.

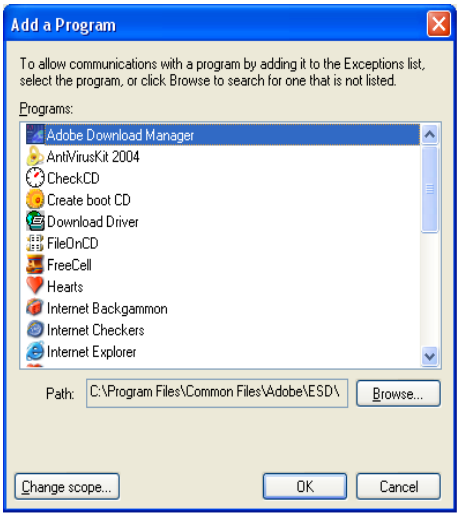


20.8.2.4 Add a program (or service) to the exception list

1. Click **Start** → **Control Panel**.
2. In the window **Control Panel** → click **Windows Security Center**.
3. Click **Windows Firewall**. A window appears → click on the **Exceptions** tab.



4. Click on **Add a Program**. This will open a dialog box.



   Click the program that you want to add, and then click **OK**. The program will appear, selected, on the **Exceptions** tab, under **Programs and Services**.

5. Click **OK**.

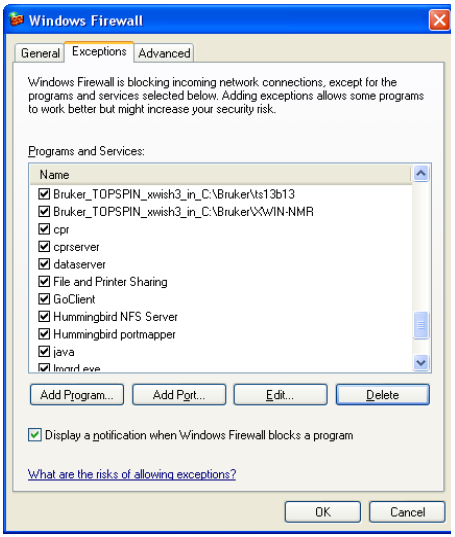
20.8.2.5 Open a Port in the exception tab

If you still do not find the program, you can open a port instead (When you open a port, remember to close it again when you are done using it.).

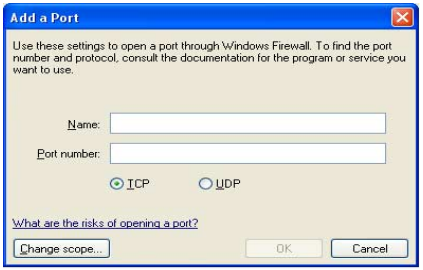
Adding an exception is preferable to opening a port because it is more secure than opening a port, because the firewall is only open while the program is waiting to receive the connection.

1. Click **Start** → **Control Panel**.
2. In the window **Control Panel** → click **Windows Security Center**.
3. Click **Windows Firewall**.

4. A window 'Windows Firewall' appears. Click on the **Exceptions** tab.



5. Click on **Add a Port**. This will open a dialog box.


Add a Port
Use these settings to open a port through Windows Firewall. To find the port number and protocol, consult the documentation for the program or service you want to use.
Name:
Port number:
TCP
UDP
What are the risks of opening a port?
Change scope...
OK
Cancel

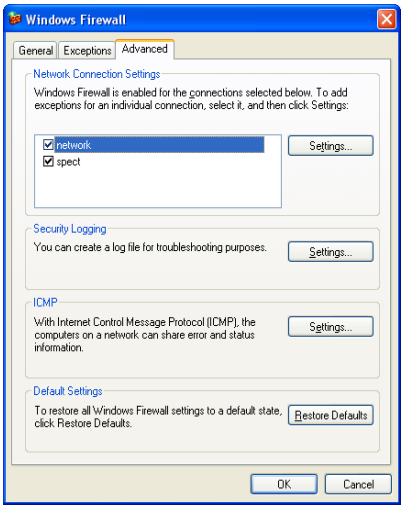
Click the program that you want to add → click **OK** → click **OK**.

20.8.2.6 Advanced Options

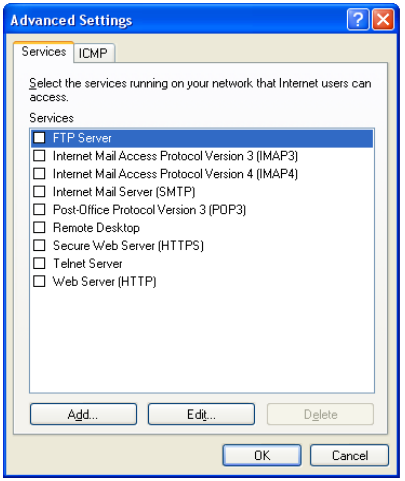
Advanced users can open ports for, and configure the scope of, individual connections to minimize opportunities for intruders to connect to a computer or network. To do this, open the Windows Firewall, select the Advanced tab and use the settings under Network Connection Settings.

1. Click **Start** → **Control Panel**.
2. In the window **Control Panel** → click **Windows Security Center**.

3. Click **Windows Firewall**.
4. A window 'Windows Firewall' appears. Click on the **Advanced** tab.


Windows Firewall
General
Exceptions
Advanced
Network Connection Settings
Windows Firewall is enabled for the connections selected below. To add exceptions for an individual connection, select it, and then click Settings:
network
spect
Settings...
Security Logging
You can create a log file for troubleshooting purposes.
Settings...
ICMP
With Internet Control Message Protocol (ICMP), the computers on a network can share error and status information.
Settings...
Default Settings
To restore all Windows Firewall settings to a default state, click Restore Defaults.
Restore Defaults
OK
Cancel

5. Click under Network Connection Settings on Settings.



6. Click **OK**.

20.8.2.7 How to disable Firewall Alerts from the Security Center

If you have installed another firewall than Windows Firewall, the Security Center

may still be able to tell you the status of that firewall and may also display an alert if it stops working.

There are some firewalls that Windows Security Center will not find, such as a hardware firewall or certain types of software firewalls. If your computer is using a hardware firewall, you should not disable Windows Firewall. If you install and run another firewall, you should turn off Windows Firewall. If you use another software firewall that Windows doesn't recognize, you may want to disable the Security Center firewall alerts.

Note: *You should only disable these alerts if you are sure that your computer is protected by a firewall. The following procedure assumes that you have already turned off Windows Firewall and that you have received an alert telling you that you do not have a firewall installed.*

20.8.2.8 How to specify a firewall that Windows does not find

1. Click **Start** → **Control Panel**.
2. Double-click **Security Center**.
3. Select **Firewall** → click **Recommendations**. (***Note****: The Recommendations button is not available when your Firewall setting is marked* ***ON***.)
4. In the **Recommendations** dialog box, select the **'I have a firewall solution that I'll monitor myself'** check box → click **OK**.

When you use this procedure, the Security Center displays your Firewall setting as Unknown, and does not send you alerts.

20.8.3 Automatic Updates

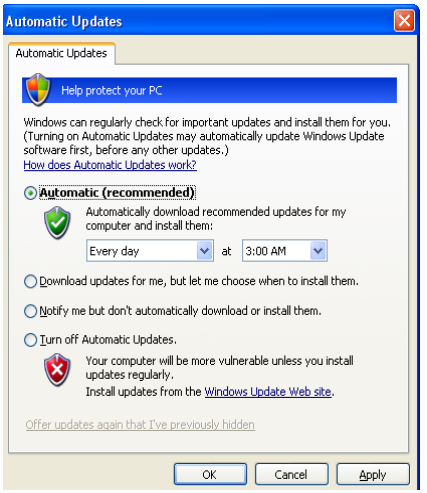
Windows Security Center allows you to easily manage security settings for Automatic Updates. When you turn on Automatic Updates, Windows routinely checks the Windows Update Web site for high-priority updates that can help protect your computer against attacks. High-priority updates include security updates, critical updates, and service packs.

20.8.3.1 How to change your Automatic Updates settings

By default, any new updates are installed each day at 3 a.m.

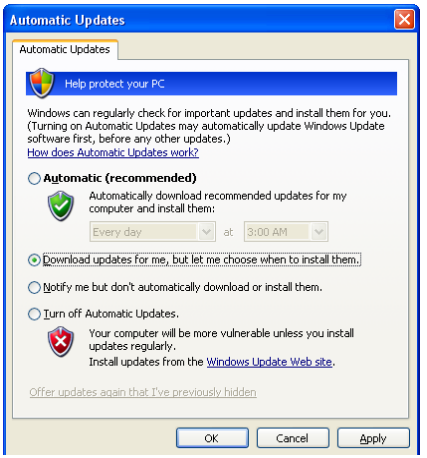
1. Click **Start** → **Control Panel**.

2. Double-click **Security Center**.
3. Under **Manage your security settings for** → click **Automatic Updates**
4. A window 'Automatic Update' will appear:.


Automatic Updates
Automatic Updates
Help protect your PC
Windows can regularly check for important updates and install them for you. (Turning on Automatic Updates may automatically update Windows Update software first, before any other updates.)
How does Automatic Updates work?
Automatic (recommended)
Automatically download recommended updates for my computer and install them:
Every day
at
3:00 AM
Download updates for me, but let me choose when to install them.
Notify me but don't automatically download or install them.
Turn off Automatic Updates.
Your computer will be more vulnerable unless you install updates regularly.
Install updates from the Windows Update Web site.
Offer updates again that I've previously hidden
OK
Cancel
Apply

The options for Automatic updates are:

- Automatic: Automatic download recommend updates for my computer and install them: e.g. 'Every day ' at '3:00 AM'
- Automatic: Download updates for me, but let me choose when to install them (recommended by Bruker BioSpin for PCs which controls spectrometer.


Automatic Updates
Automatic Updates
Help protect your PC
Windows can regularly check for important updates and install them for you. (Turning on Automatic Updates may automatically update Windows Update software first, before any other updates.)
How does Automatic Updates work?
Automatic (recommended)
Automatically download recommended updates for my computer and install them:
Every day
at
3:00 AM
Download updates for me, but let me choose when to install them.
Notify me but don't automatically download or install them.
Turn off Automatic Updates.
Your computer will be more vulnerable unless you install updates regularly.
Install updates from the Windows Update Web site.
Offer updates again that I've previously hidden
OK
Cancel
Apply

- The Updates are downloaded behind the scenes whenever you are connected to the Internet. The downloading process does not interfere with other downloads or interrupt you while you work. If you disconnect from the Internet before updates are fully downloaded, the download process will continue the next time you connect to the Internet.
- Automatic: Notify me but do not automatically download or install them.
- Turn off Automatic Updates. Your computer will be more vulnerable unless you install updates regularly. Install updates from the Windows Update Web site.

You can also visit the Windows Update Web site on a regular basis to get updates for your computer. The Web site provides the same high priority updates as Automatic Updates, but also offers optional updates that can help improve your computer's performance or add functionality to some of your programs.

Bruker BioSpin recommends to choose the option 'Download updates for me, but let me choose when to install them' because the option 'Automatic download recommend updates for my computer and install them' could cause that the PC restarts automatically after the installation of an update.

20.8.4 Antivirus

20.8.4.1 How to disable Antivirus Alertsform the Security Center

If you are running Windows XP SP2 Windows Security Center should tell you about the status of your antivirus software and display an alert if it stops working. Some antivirus programs are designed to report specific information about the program to the Security Center.

However, not all antivirus programs are designed to report to the Windows Security Center. In fact, there are some antivirus solutions that the Security Center will not detect at all. If you use an antivirus program that Windows does not recognize, and you keep it up to date and properly configured, you may want to disable the antivirus Security Center alerts.

Note *You should only disable these alerts if you are sure that your computer is protected by the full version of an up-to-date antivirus program. In addition, once you disable alerts, even if your program receives an update that makes it fully detected within Security Center, you will not receive alerts unless you clear this check box.*

20.8.4.2 How to specify an antivirus program that Windows does not find

1. Click **Start** → **Control Panel**.
2. Double-click **Security Center**.
3. In the Security Center, under **Virus Protection**, click **Recommendations**. (The Recommendations button is not available when your Virus Protection setting is marked ON.)
4. In the **Recommendations** dialog box, select the **I have antivirus software that I'll monitor myself** check box, and then click **OK**.

When you use this procedure, the Security Center displays your Virus Protection setting as Unknown, and does not send you alerts.

20.8.5 Microsoft Pop-up Blocker

With the Windows XP SP2 Internet Explorer you are able to prevent most pop-up windows from appearing over Internet pages you want to view while you are using the Internet.

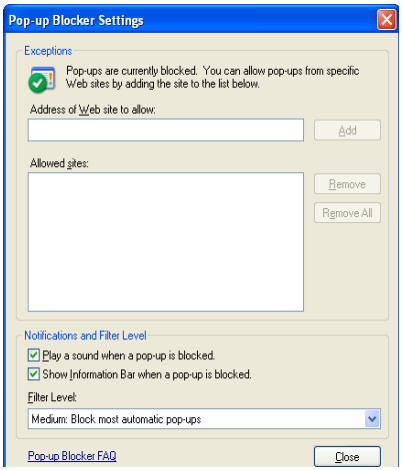
Many advertisers on the Internet use windows that pop up in the middle of your screen to display a message. They might also open when you click a link or button on a Web site, and they might open either over or under the window you wish to view. Some pop-ups are helpful. Unfortunately, some pop-up windows can contain inappropriate content or can be a way for you to accidentally download dangerous software (called spyware or adware) onto your computer.

When you install SP2, Pop-up Blocker is turned on in Internet Explorer and set to the medium setting, which means it will block most automatic pop-ups. The default settings for the pop-up blocker allow you to see pop-ups that are opened when you click a link or button on a Web site. Pop-up Blocker will also play a sound and show the Information Bar when a pop-up is blocked. You can adjust these settings so that Pop-up Blocker works the way you want it to.

20.8.5.1 How to change Pop-up Blocker settings

1. Open the Microsoft Internet Explorer.

2. On the **Tools** menu, select **Pop-up Blocker** → click **Pop-up Blocker Settings**.


Pop-up Blocker Settings
Exceptions
Pop-ups are currently blocked. You can allow pop-ups from specific Web sites by adding the site to the list below.
Address of Web site to allow:
Add
Allowed sites:
Remove
Remove All
Notifications and Filter Level
Play a sound when a pop-up is blocked.
Show Information Bar when a pop-up is blocked.
Filter Level:
Medium: Block most automatic pop-ups
Pop-up Blocker FAQ
Close

If you want to see pop-up windows from a specific Web site, type the address (or URL) of the site in the **Address of Web site to allow** box, and then click **Add**.

If you would like to temporarily allow a site to display pop-ups, click the Information Bar when it notifies you that a pop-up has been blocked → click **Temporarily Allow Pop-ups.**

20.8.5.2 How to block pop-ups when you click a link (or button) on a Web site

1. Open Internet Explorer.
2. On the **Tools** menu, select **Pop-up Blocker** → click **Pop-up Blocker Settings**.
3. Select the **High** setting in the box near the bottom of the dialog box.

Note: *If you want to see pop-ups that are blocked when you have this setting turned on, hold down the CTRL key while the window opens.*

20.8.5.3 To turn on Pop-up Blocker

1. On the **Tools** menu, select **Pop-up Blocker**.
2. Click Turn on Pop-up Blocker.

If you get similar pop-up windows no matter what sites you visit or even if you are not on the Web at all, you could have spyware, adware, or other software on your computer that's launching pop-ups. To stop these pop-ups, you will have to iden-

tify the software, then remove it or change its settings to stop it from launching pop-ups.

Pop-up Blocker will not block pop-up windows that you open deliberately by clicking a link. For example, if you were on a travel reservation site and you clicked a link to open a pop-up window containing your confirmation details, this pop-up window would not be blocked because you opened it intentionally. The Pop-up Blocker will not block some pop-ups with certain types of animated content or pop-ups from Web sites that are in two Web content zones: *Local intranet* or *Trusted sites*.

20.9 Internet Connection Firewall in Windows XP SP1

This chapter Windows XP provides internet security in the form of a firewall (Internet Connection Firewall). This feature is designed for home and small business use and provides protection for computers directly connected to the Internet. This feature is available for local area network (LAN) or dial-up connections. It also prevents scanning of ports and resources (file and printer shares) from external sources.

20.9.1 Enable Internet Connection Firewall (Windows XP SP1)

a) **Use the Network Setup Wizard to enable the Internet Connection Firewall:**

1. Run the Network Setup Wizard.
   Click **Start** → **Control Panel**, double-click **Network Connections**, and then click *Setup or change your home or small office network.*
2. The Firewall is enabled when you choose a configuration in the wizard that indicates that your computer is connected directly to the Internet.

b) **Configure the Internet Connection Firewall manually for a connection:**

1. Click **Start** → **Control Panel** → double-click **Network Connections**.
2. Right-click the connection on which you would like to enable the firewall → Click **Properties**.
3. On the **Advanced** tab, click the box to select the option to *Protect my computer or network*.
4. If you want to enable the use of some applications and services through the firewall, you need to enable them by clicking the **Settings** button.Then select the programs, protocols and services to be enabled for the firewall

configuration.

20.9.2 Disable Internet Connection Firewall (Windows XP SP1)

1. Click **Start** → **Control Panel**, double-click **Network Connections**.
2. Right-click the connection on which you would like to disable the firewall → Click **Properties**.
3. On the **Advanced** tab, click the box to clear the option to *Protect my computer or network*.

Chapter 21

Appendix

21.1 Windows XP Important Information about your PC

1. Wh*at is the Bruker BioSpin order number?*

HH _____

2. Customer details:

Name _____

Organization _____

Adr1 _____

Adr2 _____

Adr3 _____

3. Manufacturer and Type of the PC?

_____

4. Manufacturer's system ID number of the PC?

_____

5. Which service pack of Windows XP is installed: SP ____

(Shown at boot time on blue screen)

6. What type of graphics controller is installed?

_____

7. Name of NMR SUPERUSER?

_____

21.2 Some notes for the helium handling

In the TOPSPIN installation path (normally `C:\Bruker\TOPSPIN`) in the directory `...\prog\logfiles` are two files named `heliumlog` and `heliumlog.err`. The `heliumlog` saves every night at 3.00 am the actual helium level in a new line. The `heliumlog.err` documents every error during detecting the helium level.

21.2.1 Automatic notification for helium refill

1. Open a Command Prompt and enter:

- **`cd /d c:\Bruker\TOPSPIN`**
- **`notepad heliumlimit`**

type in the number (without '%') of the helium level should activate the notification, e. g. **`25`**

Click **file** → **save as ..** and save it as **`<TOPSPINHOME>\heliumlimit`**

Of course, you can also install the heliumlimit file from the Explorer. We have chosen the Command Prompt because the Explorer might add the extension `.txt` to the file `heliumlevel` which makes it unusable (see chapter 7.2.2).

2. Now you could create a command script `<TOPSPINHOME>\heliumwarn.cmd` that will be executed if the actual helium level is the same or below the entry (in %) in the file <TOPSPINHOME>\heliumlimit

E. g. it is possible to create a message window on the screen of the spectrometer PC and/or every other PC in your network (e. g. the PC of the responsible person for helium refill). You could do this in the following way:

3. Open a Command Prompt and enter:

- **`cd /d c:\Bruker\TOPSPIN`**

- **notepad heliumwarn.cmd**

type in the following text:

```
@echo off
rem -----------------------------------------------------
rem heliumwarn.cmd: example MS cmd script to send a warning
rem                 argument1=LEVEL
rem                 argument2=LIMIT
rem -----------------------------------------------------
rem  user defined variables:
rem  INSTRUMENT: is the name of the spectrometer
rem  ADDRESS   : the address where the message is sent to.
rem              type 'net help send' for details
rem -----------------------------------------------------
set INSTRUMENT='Avance-300'
set ADDRESS1=%COMPUTERNAME%
set ADDRESS2=%NMR-SUPERUSER-PC%
set ADDRESS3=%HELIUM-REFILLER-PC%
rem ------------------------------
rem  catch command line arguments:
rem ------------------------------
set MYSELF=%0
set LEVEL=%1
set LIMIT=%2
rem ---------------------------------------
rem  get the name of the spectrometer host:
rem ---------------------------------------
set HOST=%COMPUTERNAME%
rem ---------------------------
rem  prepare the email message:
rem ---------------------------
set MSG=Attention: At the magnet of the %INSTRUMENT% spec-
trometer is the heliumlevel of %LEVEL%% equal or lower than
the helium level limit of %LIMIT%%: please order liquid he-
lium and refill the helium tank. --- This message has been
```

```
sent by %MYSELF% on %HOST% to %ADDRESS1%, %ADDRESS2% and
%ADDRESS3%
rem ------------------
rem  send the message:
rem ------------------
net send %ADDRESS1% %MSG%
net send %ADDRESS2% %MSG%
net send %ADDRESS3% %MSG%
```

You have to write in your individual parameters

- replace `Avance-300` with the name of your spectrometer
- replace `NMR-SUPERUSER-PC` with the name of the PC of the NMR-Superuser
- replace `HELIUM-REFILLER-PC` with the name of the PC of the responsible person for helium refill
- Attention - the text sequence:

  `set MSG=Attention: At the magnet of the %INSTRUMENT% spectrometer is the heliumlevel of %LEVEL%%% equal or lower than the helium level limit of %LIMIT%%%: please order liquid helium and refill the helium tank. --- This message has been sent by %MYSELF% on %HOST% to %ADDRESS1%, %ADDRESS2% and %ADDRESS3%`

  had to be written in one line!

click **file** → **save as..** and save it as **`<TOPSPINHOME>\heliumwarn.cmd`**

Now the defined PC's will get an error message if the actual helium level is the same or below the entry (in %) in the file

`<TOPSPINHOME>\heliumlimit`

The notifications were sends only once but it will be activated again if the helium level is against higher than the limit.

Note that this script is only an example, if you would like to add more PC's in the notification list you had to add the respective addresses, if you like to haveless addresses you have to delete the respective entries.

21.3 Helium measurement under Windows XP Service Pack 1

On Windows XP SP1 the nightly Heliumlog does not work. The reason is a bug in Microsoft Windows XP Service Pack 1 which lets the task scheduler execute only those jobs which run under the account of the user who is currently logged on. See the article in the Microsoft knowledge base:

`http://support.microsoft.com/default.aspx?scid=kb;en-us;812400`

If there is always the same user logged on all the time, then workaround 1 can beapplied. Otherwise workaround 2 should be done.

1. Workaround 1:

The helium log runs under the local system account. Change this to the user whois always logged on:

a) Click on ***Start*** → ***Settings*** → ***Control Panel*** → 'Task Scheduler'.

b) Click twotimes on the task AT1(2,...) which runs at 3:00 AM.

c) Specify the user name besides 'Run as:' and set the password accordingly (the user must have a password!).

d) Click 'OK'.

ATTENTION:
Remove this modified task before installing a new TOPSPIN version!

2. Workaround 2:

Disable the HID-Service (Human Interface Device Access) and restart the computer.

Note: Remove this modified task before installing a new TOPSPIN version.

21.4 Script for saving important files

TOPSPIN offers a script (xwinnmr.save) for saving very important files that are not delivered by BRUKER. This script can save and extract user specific data from the TOPSPINHOME directory and puts them into a tar-file. Files that start with an "." are ignored. The script can be started as follows:

- Click on the Bruker Utilities icon on the desktop

  Bruker Utilities → ***Miscellaneous*** → ***xwinnmr.save.cmd***

- For more information open the command prompt of the Bruker Utilities

  Bruker Utilities → ***Command prompt*** and enter

  `.\prog\bin\utilities\miscellaneous\xwinnmr.save –help`

Files and directories will be saved into the special tar-file `xwin_backup.tar` which is, by default, in the directory `TOPSPINHOME/xwin_backup`.

The ***xwinnmr.save*** script saves the same files and directories as the nmr_save AU program (see chapter 8.7).

The options for ***`xwinnmr.save`*** starting from a command prompt are:
`xwinnmr.save` [-options]

- ***`help`*** additional information
- ***`path <string>`*** absolute path where backup tar-file `nmr_backup.tar` will be created (backup directory)
- ***`restore <string>`*** absolute path where backup tar-file can be found (backup directory); the target directory must also be specified! (see examples below)
- ***`replace`*** overwrite existing nmr_backup.tar file
- ***`silent`*** do not display any messages
- ***`source <string>`*** absolute path to Topspin/xwin-nmr installation that should be saved
- ***`spect <string>`*** spectrometer name (e.g. spect; default is the current name)

For safety reasons the tar-file will not be replaced by executing the ***`xwinnmr.save`*** script once again. So if you like to use the script several times, you have to move the `xwin_backup.tar` file from the directory `TOPSPINHOME/xwin_backup` on a backup medium (floppy, CD ...) and then start the script once again or you have to use the ’replace’ option.

21.5 Where Do I Find What?

If you cannot find the required information in this manual, please check the manuals listed below.

Further useful information you can also find in the Release Letter for the respective TOPSPIN version.

- TOPSPIN Users Guide
  Window handling, diplaying data, interactive data manipulation, user interface related items.
- Acquisition Reference
  Description of all acquisition commands, parameters and files.
- Processing Reference
  Description of all processing commands, parameters and files.
- AU Reference
  How to write AU programs. Description of all AU macros, functions and variables. List of Bruker AU programs.
- TOPSPIN PLOT EDITOR
  Printing and plotting of data sets.
- NMR-SIM Experiment Simulator
  Simulation of NMR experiments.
- ICON-NMR Automation Interface
  Comprehensive user interface, tailormade for all your laboratory management and control needs.

For further manuals please refer to:

- TOPSPIN → **Help**
- http://www.bruker-biospin.de/NMR/nmrsoftw/passwd/docu/index.html
- NMR-GUIDE

Chapter 22

Bruker BioSpin addresses

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Silberstreifen
D-76287 Rheinstetten
Tel: (++49) (721) 5161 455
Fax: (++49) (721) 5161 943

http://www.bruker-biospin.de

ftp server: ftp.bruker.de

Email: nmr@bruker-biospin.de (sales)
mbu@bruker.de (service)
applik@bruker.de (application)
nmr-software-support@bruker-biospin.de (software)
license@bruker.de (licenses)

USA

```
Bruker BioSpin Corporation
15 Fortune Drive
Manning Road
Billerica, MA. 01821-3991

Tel: (++1)(978) 667 9580 5195 (center)
     (++1)(978) 667 9580 5444 (application)
Fax: (++1)(978) 667 6168 (center)
     (++1)(978) 667 2955 (application)

http://www.bruker-biospin.com
ftp server: ftp.bruker.com

Email: applab@bruker.com
       center@bruker.com
       software@bruker.com
```

Switzerland

```
Bruker BioSpin AG
Industriestraße 26
CH-8117 Fällanden

Tel: (++41)(1) 8 25 91 11
Fax: (++41)(1) 8 25 96 96

web server: www.bruker.ch
E-Mail: epweb@bruker.ch
        all_ap@bruker.ch
```

France

```
Bruker BioSpin S.A.
34, rue de l'industrie
F-67166 Wissembourg/Cedex

Tel: (++33)(3) 88 73 68 00
Fax: (++33)(3) 88 73 68 79

web server: www.bruker.fr
E-Mail: support-rmn@bruker.fr (customer support)
```

England

Bruker BioSpin LTD.
Banner lane
Coventry CV4 9GH
Tel: (++44)(2476) 855200
Fax: (++44)(2476) 465317

web server: www.bruker.co.uk

Email:service@bruker.co.uk
apps@bruker.co.uk

Our webpage

http://www.bruker-biospin.de/NMR/about/offices/index.html

- provides contact adresses of our facilities and offices worldwide

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